Valproic Acid

Other names:	(n-C3H7)2CHCOOH
	2,2-Di-n-propylacetic acid
	2-Propylpentanoic acid
	2-Propylvaleric acid
	2-n-Propyl-n-valeric acid
	4-Heptanecarboxylic acid
	44089
	Abbott 44090
	Acetic acid, dipropyl-
	DPA
	Depakene
	Depakine
	Di-n-propylacetic acid
	Di-n-propylessigsaure
	Dipropylacetic acid
	Divalproex
	Ergenyl
	Kyselina 2-propylvalerova
	Mylproin
	NSC 93819
	Pentanoic acid, 2-propyl-
	Propylvaleric acid
	Valeric acid, 2-propyl-
	n-DPA
	n-Dipropylacetic acid
Inchi:	InChI=1S/C8H16O2/c1-3-5-7(6-4-2)8(9)10/h7H,3-6H2,1-2H3,(H,9,10)
InchiKey:	NIJJYAXOARWZEE-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	CCCC(CCC)C(=O)O
Mol. weight [g/mol]:	144.21
CAS:	99-66-1

Physical Properties

Property code	Value	Unit	Source
gf	-251.70	kJ/mol	Joback Method
hf	-478.54	kJ/mol	Joback Method

hfus	74.80	kJ/mol	Vaporization Enthalpy and Vapor Pressure of Valproic Acid by Correlation Gas Chromatography
hvap	56.44	kJ/mol	Joback Method
log10ws	-1.86		Aqueous Solubility Prediction Method
logp	2.287		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	3009.03	kPa	Joback Method
rinpol	1116.00		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	1084.00		NIST Webbook
tb	493.20	K	NIST Webbook
tc	700.14	K	Joback Method
tf	275.67	K	Joback Method
vc	0.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.75	J/mol×K	528.05	Joback Method
cpg	360.77	J/mol×K	671.46	Joback Method
cpg	351.46	J/mol×K	642.78	Joback Method
cpg	341.71	J/mol×K	614.10	Joback Method
cpg	331.52	J/mol×K	585.41	Joback Method
cpg	320.87	J/mol×K	556.73	Joback Method
cpg	369.66	J/mol×K	700.14	Joback Method
dvisc	0.0001397	Pa×s	528.05	Joback Method
dvisc	0.0002310	Pa×s	485.99	Joback Method
dvisc	0.0004201	Pa×s	443.92	Joback Method
dvisc	0.0008658	Pa×s	401.86	Joback Method
dvisc	0.0021132	Pa×s	359.80	Joback Method
dvisc	0.0065326	Pa×s	317.73	Joback Method
dvisc	0.0284980	Pa×s	275.67	Joback Method

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.01765e+01
Coeff. B	-6.30193e+03
Coeff. C	-8.81420e+01
Temperature range (K), min.	405.00
Temperature range (K), max.	512.09

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C99661&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Vaporization Enthalpy and Vapor Pressure of Valproic Acid by Correlation Gas Chromatography:	https://www.doi.org/10.1021/je3003767

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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