

Meso-2,3-diethylbutanedioic acid

Inchi:	InChI=1S/C8H14O4/c1-3-5(7(9)10)6(4-2)8(11)12/h5-6H,3-4H2,1-2H3,(H,9,10)(H,11,12)/t
InchiKey:	KJXMXCRSMLOXBM-OLQVQODUSA-N
Formula:	C8H14O4
SMILES:	CCC(C(=O)O)C(CC)C(=O)O
Mol. weight [g/mol]:	174.19
CAS:	35392-80-4

Physical Properties

Property code	Value	Unit	Source
chs	-4130.00	kJ/mol	NIST Webbook
gf	-519.88	kJ/mol	Joback Method
hf	-748.63	kJ/mol	Joback Method
hfus	20.80	kJ/mol	Joback Method
hvap	79.48	kJ/mol	Joback Method
log10ws	-0.89		Crippen Method
logp	1.208		Crippen Method
mcvol	138.460	ml/mol	McGowan Method
pc	3628.97	kPa	Joback Method
tb	673.66	K	Joback Method
tc	851.26	K	Joback Method
tf	371.42	K	Joback Method
vc	0.521	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.77	J/molxK	673.66	Joback Method
cpg	382.66	J/molxK	703.26	Joback Method
cpg	391.09	J/molxK	732.86	Joback Method
cpg	399.07	J/molxK	762.46	Joback Method
cpg	406.62	J/molxK	792.06	Joback Method
cpg	413.74	J/molxK	821.66	Joback Method
cpg	420.46	J/molxK	851.26	Joback Method
dvisc	0.0094190	Paxs	371.42	Joback Method

dvisc	0.0018445	Paxs	421.79	Joback Method
dvisc	0.0005115	Paxs	472.17	Joback Method
dvisc	0.0001816	Paxs	522.54	Joback Method
dvisc	0.0000774	Paxs	572.91	Joback Method
dvisc	0.0000378	Paxs	623.29	Joback Method
dvisc	0.0000206	Paxs	673.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35392804&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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