Butanoic acid, heptafluoro-

Other names:	Butanoic acid, 2,2,3,3,4,4,4-heptafluoro-
	Butyric acid, heptafluoro-
	Heptafluoro-1-butanoic acid
	Heptafluoro-n-butyric acid
	Heptafluorobutanoic acid
	Heptafluorobutyric acid
	Kyselina heptafluormaselna
	NSC 820
	Perfluorobutanoic acid
	Perfluorobutyric acid
	Perfluoropropanecarboxylic acid
Inchi:	InChI=1S/C4HF7O2/c5-2(6,1(12)13)3(7,8)4(9,10)11/h(H,12,13)
InchiKey:	YPJUNDFVDDCYIH-UHFFFAOYSA-N
Formula:	C4HF7O2
SMILES:	O=C(O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	214.04
CAS:	375-22-4

Physical Properties

Property code	Value	Unit	Source
gf	-1638.09	kJ/mol	Joback Method
hf	-1789.72	kJ/mol	Joback Method
hfus	11.12	kJ/mol	Joback Method
hvap	38.32	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.904		Crippen Method
mcvol	87.050	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
rinpol	863.00		NIST Webbook
rinpol	863.00		NIST Webbook
tb	393.00 ± 1.00	K	NIST Webbook
tc	568.58	K	Joback Method
tf	256.98	K	Joback Method
vc	0.378	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.91	J/mol×K	422.17	Joback Method
cpg	219.97	J/mol×K	446.57	Joback Method
cpg	226.49	J/mol×K	470.97	Joback Method
cpg	232.52	J/mol×K	495.38	Joback Method
cpg	238.06	J/mol×K	519.78	Joback Method
cpg	243.15	J/mol×K	544.18	Joback Method
cpg	247.82	J/mol×K	568.58	Joback Method
hvapt	50.10 ± 0.20	kJ/mol	368.00	NIST Webbook
hvapt	45.90 ± 0.20	kJ/mol	368.00	NIST Webbook
hvapt	41.00 ± 0.50	kJ/mol	368.00	NIST Webbook
hvapt	47.80	kJ/mol	411.00	NIST Webbook
hvapt	47.30	kJ/mol	373.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	393.20	K	101.00	NIST Webbook
tbrp	1028.00	K	16.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.90175e+01
Coeff. B	-5.67545e+03
Temperature range (K), min.	303.01
Temperature range (K), max.	414.08

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C375224&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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
hvapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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