

Tridecafluoroheptanoic acid

Other names:	Perfluoroheptanoic acid Heptanoic acid, tridecafluoro-
Inchi:	InChI=1S/C7HF13O2/c8-2(9,1(21)22)3(10,11)4(12,13)5(14,15)6(16,17)7(18,19)20/h(H,2
InchiKey:	ZWBAMYVPMDSJGQ-UHFFFAOYSA-N
Formula:	C7HF13O2
SMILES:	O=C(O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	364.06
CAS:	375-85-9

Physical Properties

Property code	Value	Unit	Source
gf	-2773.17	kJ/mol	Joback Method
hf	-3054.55	kJ/mol	Joback Method
hfus	15.13	kJ/mol	Joback Method
hvap	36.20	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.810		Crippen Method
mcvol	139.940	ml/mol	McGowan Method
pc	2054.89	kPa	Joback Method
tb	476.74	K	Joback Method
tc	609.45	K	Joback Method
tf	301.59	K	Joback Method
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	392.19	J/mol×K	476.74	Joback Method
cpg	401.52	J/mol×K	498.86	Joback Method
cpg	410.11	J/mol×K	520.98	Joback Method
cpg	418.01	J/mol×K	543.09	Joback Method
cpg	425.25	J/mol×K	565.21	Joback Method
cpg	431.87	J/mol×K	587.33	Joback Method
cpg	437.90	J/mol×K	609.45	Joback Method

hvapt	61.40 ± 0.30	kJ/mol	422.00	NIST Webbook
hvapt	55.50 ± 0.30	kJ/mol	422.00	NIST Webbook
hvapt	48.70 ± 0.70	kJ/mol	422.00	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C375859&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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