Heptafluorobutyric anhydride

Other names:	Heptafluorobutanoic anhydride
	Perfluorobutyric anhydride
	Heptafluoro-n-butyric anhydride
	Butanoic acid, heptafluoro-, anhydride
Inchi:	InChI=1S/C8F14O3/c9-3(10,5(13,14)7(17,18)19)1(23)25-2(24)4(11,12)6(15,16)8(20,21)2
InchiKey:	UFFSXJKVKBQEHC-UHFFFAOYSA-N
Formula:	C8F14O3
SMILES:	O=C(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	410.06
CAS:	336-59-4

Physical Properties

Property code	Value	Unit	Source
gf	-3056.66	kJ/mol	Joback Method
hf	-3363.87	kJ/mol	Joback Method
hfus	19.50	kJ/mol	Joback Method
hvap	30.09	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.722		Crippen Method
mcvol	157.370	ml/mol	McGowan Method
pc	1746.28	kPa	Joback Method
tb	382.20	K	NIST Webbook
tb	379.50 ± 0.50	K	NIST Webbook
tb	382.00 ± 1.00	K	NIST Webbook
tc	619.92	K	Joback Method
tf	324.79	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.28	J/mol×K	483.00	Joback Method
cpg	443.32	J/mol×K	505.82	Joback Method
cpg	452.61	J/mol×K	528.64	Joback Method

cpg	461.17	J/mol×K	551.46	Joback Method
cpg	469.04	J/mol×K	574.28	Joback Method
cpg	476.25	J/mol×K	597.10	Joback Method
cpg	482.86	J/mol×K	619.92	Joback Method

Sources

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=C336594&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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