Heptafluorobutyric acid, 2-methylpropyl ester

Other names: Heptafluorobutyric acid, isobutyl ester
Inchi: InChI=1S/C8H9F7O2/c1-4(2)3-17-5(16)6(9,10)7(11,12)8(13,14)15/h4H,3H2,1-2H3
InchiKey: PTTNLWHRSGDGJX-UHFFFAOYSA-N
Formula: C8H9F7O2
SMILES: CC(C)COC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 270.14
CAS: 49669-71-8

Physical Properties

Property code	Value	Unit	Source
gf	-1575.03	kJ/mol	Joback Method
hf	-1857.55	kJ/mol	Joback Method
hfus	15.06	kJ/mol	Joback Method
hvap	32.56	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	3.018		Crippen Method
mcvol	143.410	ml/mol	McGowan Method
pc	2085.03	kPa	Joback Method
rinpol	711.00		NIST Webbook
tb	443.49	K	Joback Method
tc	594.62	K	Joback Method
tf	248.47	K	Joback Method
vc	0.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.91	J/mol×K	443.49	Joback Method
cpg	356.88	J/mol×K	468.68	Joback Method
cpg	368.17	J/mol×K	493.87	Joback Method
cpg	378.83	J/mol×K	519.06	Joback Method
cpg	388.86	J/mol×K	544.24	Joback Method
cpg	398.30	J/mol×K	569.43	Joback Method
cpg	407.18	J/mol×K	594.62	Joback Method

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=C49669718&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume