Butyric acid, heptafluoro-, butyl ester

Other names:	Heptafluorobutyric acid, n-butyl ester
	Butyl heptafluorobutyrate
	Butyl 2,2,3,3,4,4,4-heptafluorobutanoate
	1-Butanol, heptafluorobutyrate
	Butyl perfluorobutyrate
	2,2,3,3,4,4,4-Heptafluoro-butyric acid butyl ester
	Butanoic acid, heptafluoro, butyl ester
	Butyl heptafluorobutanoate
	Heptafluorobutyric acid, butyl ester
Inchi:	InChI=1S/C8H9F7O2/c1-2-3-4-17-5(16)6(9,10)7(11,12)8(13,14)15/h2-4H2,1H3
InchiKey:	YDXXJZKOOOJVEE-UHFFFAOYSA-N
Formula:	C8H9F7O2
SMILES:	CCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	270.14
CAS:	1559-07-5

Physical Properties

Property code	Value	Unit	Source
gf	-1572.59	kJ/mol	Joback Method
hf	-1852.27	kJ/mol	Joback Method
hfus	18.58	kJ/mol	Joback Method
hvap	32.95	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.163		Crippen Method
mcvol	143.410	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinpol	737.00		NIST Webbook
rinpol	735.00		NIST Webbook
rinpol	734.60		NIST Webbook
rinpol	748.00		NIST Webbook
rinpol	777.30		NIST Webbook
ripol	730.00		NIST Webbook
tb	443.93	K	Joback Method
tc	592.16	K	Joback Method
tf	263.47	K	Joback Method
vc	0.601	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.85	J/mol×K	443.93	Joback Method
cpg	356.52	J/mol×K	468.64	Joback Method
cpg	367.55	J/mol×K	493.34	Joback Method
cpg	377.96	J/mol×K	518.05	Joback Method
cpg	387.78	J/mol×K	542.75	Joback Method
cpg	397.03	J/mol×K	567.46	Joback Method
cpg	405.74	J/mol×K	592.16	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1559075&Units=SI
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
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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume