Heptafluorobutyric acid, heptyl ester

Other names: Heptyl heptafluorobutanoate
Butanoic acid, heptafluoro, heptyl ester
Heptyl heptafluorobutyrate
Inchi: InChI=1S/C11H15F7O2/c1-2-3-4-5-6-7-20-8(19)9(12,13)10(14,15)11(16,17)18/h2-7H2,1
InchiKey: DUJUFOWMNOQMBF-UHFFFAOYSA-N
Formula: C11H15F7O2
SMILES: CCCCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 312.22
CAS: 866-19-3

Physical Properties

Property code	Value	Unit	Source
gf	-1547.33	kJ/mol	Joback Method
hf	-1914.19	kJ/mol	Joback Method
hfus	26.35	kJ/mol	Joback Method
hvap	39.63	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.333		Crippen Method
mcvol	185.680	ml/mol	McGowan Method
pc	1618.07	kPa	Joback Method
rinpol	1010.00		NIST Webbook
rinpol	1026.00		NIST Webbook
rinpol	1038.80		NIST Webbook
rinpol	1017.00		NIST Webbook
ripol	1025.00		NIST Webbook
ripol	1016.00		NIST Webbook
tb	512.57	K	Joback Method
tc	660.66	K	Joback Method
tf	297.28	K	Joback Method
vc	0.768	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	480.99	J/mol×K	512.57	Joback Method
cpg	494.46	J/mol×K	537.25	Joback Method
cpg	507.23	J/mol×K	561.93	Joback Method
cpg	519.34	J/mol×K	586.62	Joback Method
cpg	530.79	J/mol×K	611.30	Joback Method
cpg	541.64	J/mol×K	635.98	Joback Method
cpg	551.89	J/mol×K	660.66	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=C866193&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume