Heptadecyl heptafluorobutyrate

Other names:	Heptadecyl 2,2,3,3,4,4,4-heptafluorobutanoate
	1-Heptadecanol, heptafluorobutyrate
	Heptadecyl perfluorobutyrate
	Heptafluorobutyric acid, heptadecyl ester
Inchi:	InChI=1S/C21H35F7O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-30-18(29)19(22,23
InchiKey:	JMANSDFHCFBZBM-UHFFFAOYSA-N
Formula:	C21H35F7O2
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	452.49
CAS:	959085-66-6

Physical Properties

Property code	Value	Unit	Source
gf	-1463.13	kJ/mol	Joback Method
hf	-2120.59	kJ/mol	Joback Method
hfus	52.25	kJ/mol	Joback Method
hvap	61.89	kJ/mol	Joback Method
log10ws	-8.77		Crippen Method
logp	8.234		Crippen Method
mcvol	326.580	ml/mol	McGowan Method
pc	842.11	kPa	Joback Method
rinpol	1938.00		NIST Webbook
tb	741.37	K	Joback Method
tc	907.84	K	Joback Method
tf	409.98	K	Joback Method
vc	1.329	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1026.37	J/mol×K	741.37	Joback Method
cpg	1044.61	J/mol×K	769.12	Joback Method
cpg	1061.89	J/mol×K	796.86	Joback Method
cpg	1078.25	J/mol×K	824.61	Joback Method

cpg	1093.76	J/mol×K	852.35	Joback Method
cpg	1108.47	J/mol×K	880.10	Joback Method
cpg	1122.43	J/mol×K	907.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C959085666&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume