Octacosyl heptafluorobutyrate

Other names:	Octacosyl 2,2,3,3,4,4,4-heptafluorobutanoate
	1-Octacosanol, heptafluorobutyrate
	Octacosyl perfluorobutyrate
Inchi:	InChI=1S/C32H57F7O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23
InchiKey:	LUZCOQCDQZIGAN-UHFFFAOYSA-N
Formula:	C32H57F7O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	606.78

Physical Properties

Property code	Value	Unit	Source
gf	-1370.51	kJ/mol	Joback Method
hf	-2347.63	kJ/mol	Joback Method
hfus	80.74	kJ/mol	Joback Method
hvap	86.37	kJ/mol	Joback Method
log10ws	-13.37		Crippen Method
logp	12.525		Crippen Method
mcvol	481.570	ml/mol	McGowan Method
pc	493.39	kPa	Joback Method
rinpol	2983.40		NIST Webbook
rinpol	2983.40		NIST Webbook
tb	993.05	K	Joback Method
tc	1274.81	K	Joback Method
tf	533.95	K	Joback Method
vc	1.944	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1727.05	J/mol×K	993.05	Joback Method
cpg	1757.23	J/mol×K	1040.01	Joback Method
cpg	1785.34	J/mol×K	1086.97	Joback Method
cpg	1811.74	J/mol×K	1133.93	Joback Method
cpg	1836.77	J/mol×K	1180.89	Joback Method

cpg	1860.78	J/mol×K	1227.85	Joback Method
cpg	1884.12	J/mol×K	1274.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U351836&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