Hexacosyl heptafluorobutyrate

Other names:	Hexacosyl 2,2,3,3,4,4,4-heptafluorobutanoate
	1-Hexacosanol, heptafluorobutyrate
	Hexacosyl perfluorobutyrate
Inchi:	InChI=1S/C30H53F7O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23
InchiKey:	QHZFIZAXWYXCPT-UHFFFAOYSA-N
Formula:	C30H53F7O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	578.73

Physical Properties

Property code	Value	Unit	Source
gf	-1387.35	kJ/mol	Joback Method
hf	-2306.35	kJ/mol	Joback Method
hfus	75.56	kJ/mol	Joback Method
hvap	81.92	kJ/mol	Joback Method
log10ws	-12.53		Crippen Method
logp	11.745		Crippen Method
mcvol	453.390	ml/mol	McGowan Method
pc	538.33	kPa	Joback Method
rinpol	2792.10		NIST Webbook
tb	947.29	K	Joback Method
tc	1195.69	K	Joback Method
tf	511.41	K	Joback Method
vc	1.833	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1594.55	J/mol×K	947.29	Joback Method
cpg	1621.45	J/mol×K	988.69	Joback Method
cpg	1646.57	J/mol×K	1030.09	Joback Method
cpg	1670.15	J/mol×K	1071.49	Joback Method
cpg	1692.42	J/mol×K	1112.89	Joback Method
cpg	1713.60	J/mol×K	1154.29	Joback Method

cpg	1733.93	J/mol×K	1195.69	Joback Method

Sources

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=U351833&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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