Heptacosyl heptafluorobutyrate

Other names:	Heptacosyl 2,2,3,3,4,4,4-heptafluorobutanoate
	1-Heptacosanol, heptafluorobutyrate
	Heptacosyl perfluorobutyrate
Inchi:	InChI=1S/C31H55F7O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23
InchiKey:	FWXWZVBDHSMBHR-UHFFFAOYSA-N
Formula:	C31H55F7O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	592.76

Physical Properties

Property code	Value	Unit	Source
gf	-1378.93	kJ/mol	Joback Method
hf	-2326.99	kJ/mol	Joback Method
hfus	78.15	kJ/mol	Joback Method
hvap	84.15	kJ/mol	Joback Method
log10ws	-12.95		Crippen Method
logp	12.135		Crippen Method
mcvol	467.480	ml/mol	McGowan Method
pc	515.12	kPa	Joback Method
rinpol	2891.60		NIST Webbook
rinpol	2891.60		NIST Webbook
tb	970.17	K	Joback Method
tc	1234.36	K	Joback Method
tf	522.68	K	Joback Method
vc	1.889	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1660.57	J/mol×K	970.17	Joback Method
cpg	1689.02	J/mol×K	1014.20	Joback Method
cpg	1715.56	J/mol×K	1058.23	Joback Method
cpg	1740.46	J/mol×K	1102.26	Joback Method
cpg	1764.02	J/mol×K	1146.30	Joback Method

cpg	1786.50	J/mol×K	1190.33	Joback Method
cpg	1808.19	J/mol×K	1234.36	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=U351840&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume