Hexacosyl pentafluoropropionate

Other names: Hexacosyl 2,2,3,3,3-pentafluoropropanoate
1-Hexacosanol, pentafluoropropionate
Inchi: InChI=1S/C29H53F5O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23
InchiKey: PAKFICMSOWIPAA-UHFFFAOYSA-N
Formula: C29H53F5O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 528.72

Physical Properties

Property code	Value	Unit	Source
gf	-1008.99	kJ/mol	Joback Method
hf	-1884.74	kJ/mol	Joback Method
hfus	74.23	kJ/mol	Joback Method
hvap	82.63	kJ/mol	Joback Method
log10ws	-11.80		Crippen Method
logp	11.110		Crippen Method
mcvol	435.760	ml/mol	McGowan Method
pc	582.60	kPa	Joback Method
rinpol	2769.50		NIST Webbook
rinpol	2769.50		NIST Webbook
tb	929.10	K	Joback Method
tc	1160.69	K	Joback Method
tf	496.54	K	Joback Method
vc	1.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1515.63	J/mol×K	929.10	Joback Method
cpg	1541.19	J/mol×K	967.70	Joback Method
cpg	1565.06	J/mol×K	1006.30	Joback Method
cpg	1587.39	J/mol×K	1044.89	Joback Method
cpg	1608.34	J/mol×K	1083.49	Joback Method
cpg	1628.06	J/mol×K	1122.09	Joback Method

cpg	1646.70	J/mol×K	1160.69	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=U351812&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