Eicosyl pentafluoropropionate

Other names: Eicosyl 2,2,3,3,3-pentafluoropropanoate
1-Eicosanol, pentafluoropropionate
Inchi: InChI=1S/C23H41F5O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-30-21(29
InchiKey: JGDSVZMRPCCVOK-UHFFFAOYSA-N
Formula: C23H41F5O2
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 444.56

Physical Properties

Property code	Value	Unit	Source
gf	-1059.51	kJ/mol	Joback Method
hf	-1760.90	kJ/mol	Joback Method
hfus	58.68	kJ/mol	Joback Method
hvap	69.27	kJ/mol	Joback Method
log10ws	-9.29		Crippen Method
logp	8.769		Crippen Method
mcvol	351.220	ml/mol	McGowan Method
pc	785.95	kPa	Joback Method
rinpol	2198.50		NIST Webbook
tb	791.82	K	Joback Method
tc	969.66	K	Joback Method
tf	428.92	K	Joback Method
vc	1.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1132.07	J/mol×K	791.82	Joback Method
cpg	1152.04	J/mol×K	821.46	Joback Method
cpg	1170.94	J/mol×K	851.10	Joback Method
cpg	1188.83	J/mol×K	880.74	Joback Method
cpg	1205.76	J/mol×K	910.38	Joback Method
cpg	1221.79	J/mol×K	940.02	Joback Method
cpg	1236.99	J/mol×K	969.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U351808&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

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