Eicosyl heptafluorobutyrate

Other names:	Eicosyl 2,2,3,3,4,4,4-heptafluorobutanoate
	1-Eicosanol, heptafluorobutyrate
	Eicosyl perfluorobutyrate
Inchi:	InChI=1S/C24H41F7O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-33-21(32
InchiKey:	GZZZUVCGQHMCOJ-UHFFFAOYSA-N
Formula:	C24H41F7O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	494.57

Physical Properties

Property code	Value	Unit	Source
gf	-1437.87	kJ/mol	Joback Method
hf	-2182.51	kJ/mol	Joback Method
hfus	60.02	kJ/mol	Joback Method
hvap	68.57	kJ/mol	Joback Method
log10ws	-10.02		Crippen Method
logp	9.404		Crippen Method
mcvol	368.850	ml/mol	McGowan Method
pc	717.22	kPa	Joback Method
rinpol	2225.80		NIST Webbook
tb	810.01	K	Joback Method
tc	993.96	K	Joback Method
tf	443.79	K	Joback Method
vc	1.496	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1209.78	J/mol×K	810.01	Joback Method
cpg	1230.07	J/mol×K	840.67	Joback Method
cpg	1249.22	J/mol×K	871.33	Joback Method
cpg	1267.31	J/mol×K	901.99	Joback Method
cpg	1284.41	J/mol×K	932.64	Joback Method
cpg	1300.61	J/mol×K	963.30	Joback Method

cpg	1315.99	J/mol×K	993.96	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=U351835&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

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