Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl 5-methoxy-3-methylpent-2-yl ester

Inchi: InChI=1S/C16H22F8O5/c1-9(6-7-27-3)10(2)29-12(26)5-4-11(25)28-8-14(19,20)16(23,24)
InchiKey: MKJSGFPGCBJTEI-UHFFFAOYSA-N
Formula: C16H22F8O5
SMILES: COCCC(C)C(C)OC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F
Mol. weight [g/mol]: 446.33

Physical Properties

Property code	Value	Unit	Source
gf	-2046.28	kJ/mol	Joback Method
hf	-2606.36	kJ/mol	Joback Method
hfus	35.79	kJ/mol	Joback Method
hvap	60.34	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	4.085		Crippen Method
mcvol	271.210	ml/mol	McGowan Method
pc	1142.89	kPa	Joback Method
rinpol	1744.00		NIST Webbook
rinpol	1744.00		NIST Webbook
tb	723.63	K	Joback Method
tc	890.01	K	Joback Method
tf	403.61	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	832.96	J/mol×K	723.63	Joback Method
cpg	847.23	J/mol×K	751.36	Joback Method
cpg	860.65	J/mol×K	779.09	Joback Method
cpg	873.25	J/mol×K	806.82	Joback Method
cpg	885.06	J/mol×K	834.55	Joback Method
cpg	896.11	J/mol×K	862.28	Joback Method
cpg	906.43	J/mol×K	890.01	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=U389666&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