Diethylmalonic acid, 2,2,3,3,3-pentafluoropropyl undecyl ester

Inchi: InChI=1S/C21H35F5O4/c1-4-7-8-9-10-11-12-13-14-15-29-17(27)19(5-2,6-3)18(28)30-16
InchiKey: UMZABEOHNMPJEF-UHFFFAOYSA-N
Formula: C21H35F5O4
SMILES: CCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(F)(F)C(F)(F)F
Mol. weight [g/mol]: 446.49

Physical Properties

Property code	Value	Unit	Source
gf	-1307.43	kJ/mol	Joback Method
hf	-1973.17	kJ/mol	Joback Method
hfus	48.88	kJ/mol	Joback Method
hvap	72.68	kJ/mol	Joback Method
log10ws	-7.07		Crippen Method
logp	6.608		Crippen Method
mcvol	330.480	ml/mol	McGowan Method
pc	912.73	kPa	Joback Method
rinpol	1918.00		NIST Webbook
rinpol	1918.00		NIST Webbook
tb	819.12	K	Joback Method
tc	1002.94	K	Joback Method
tf	480.96	K	Joback Method
vc	1.317	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1069.55	J/mol×K	819.12	Joback Method
cpg	1086.80	J/mol×K	849.76	Joback Method
cpg	1103.01	J/mol×K	880.39	Joback Method
cpg	1118.25	J/mol×K	911.03	Joback Method
cpg	1132.57	J/mol×K	941.67	Joback Method
cpg	1146.04	J/mol×K	972.30	Joback Method
cpg	1158.72	J/mol×K	1002.94	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=U370848&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