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

Inchi: InChI=1S/C28H49F5O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-36-24(34)2

InchiKey: MNESARZGSXRYSX-UHFFFAOYSA-N

Formula: C28H49F5O4

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(F)(F)C(F)(F)F

Mol. weight [g/mol]: 544.68

Physical Properties

Property code	Value	Unit	Source
gf	-1248.49	kJ/mol	Joback Method
hf	-2117.65	kJ/mol	Joback Method
hfus	67.01	kJ/mol	Joback Method
hvap	88.26	kJ/mol	Joback Method
log10ws	-10.00		Crippen Method
logp	9.338		Crippen Method
mcvol	429.110	ml/mol	McGowan Method
pc	630.66	kPa	Joback Method
rinpol	2596.00		NIST Webbook
tb	979.28	K	Joback Method
tc	1221.54	K	Joback Method
tf	559.85	K	Joback Method
vc	1.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1506.90	J/mol×K	979.28	Joback Method
cpg	1529.42	J/mol×K	1019.66	Joback Method
cpg	1550.32	J/mol×K	1060.03	Joback Method
cpg	1569.78	J/mol×K	1100.41	Joback Method
cpg	1587.95	J/mol×K	1140.79	Joback Method
cpg	1605.03	J/mol×K	1181.16	Joback Method
cpg	1621.17	J/mol×K	1221.54	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=U370855&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