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

Inchi: InChI=1S/C30H53F5O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-38-2

InchiKey: RLOJCCFPAFZPSM-UHFFFAOYSA-N

Formula: C30H53F5O4

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

Mol. weight [g/mol]: 572.73

Physical Properties

Property code	Value	Unit	Source
gf	-1231.65	kJ/mol	Joback Method
hf	-2158.93	kJ/mol	Joback Method
hfus	72.19	kJ/mol	Joback Method
hvap	92.71	kJ/mol	Joback Method
log10ws	-10.84		Crippen Method
logp	10.119		Crippen Method
mcvol	457.290	ml/mol	McGowan Method
pc	573.98	kPa	Joback Method
rinpol	2785.00		NIST Webbook
rinpol	2785.00		NIST Webbook
tb	1025.04	K	Joback Method
tc	1295.96	K	Joback Method
tf	582.39	K	Joback Method
vc	1.821	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1636.55	J/mol×K	1025.04	Joback Method
cpg	1661.43	J/mol×K	1070.19	Joback Method
cpg	1684.41	J/mol×K	1115.35	Joback Method
cpg	1705.76	J/mol×K	1160.50	Joback Method
cpg	1725.73	J/mol×K	1205.65	Joback Method
cpg	1744.58	J/mol×K	1250.81	Joback Method
cpg	1762.56	J/mol×K	1295.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370856&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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