Diethylmalonic acid, tetradecyl 1,1,1-trifluoroprop-2-yl ester

Inchi: InChI=1S/C24H43F3O4/c1-5-8-9-10-11-12-13-14-15-16-17-18-19-30-21(28)23(6-2,7-3)22(29)31-20(4)24(25,26)27

InchiKey: FAPUMFFKIYBLGC-UHFFFAOYSA-N

Formula: C24H43F3O4

SMILES: CCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OC(C)C(F)(F)F

Mol. weight [g/mol]: 452.59

Physical Properties

Property code	Value	Unit	Source
gf	-897.83	kJ/mol	Joback Method
hf	-1639.40	kJ/mol	Joback Method
hfus	54.38	kJ/mol	Joback Method
hvap	81.90	kJ/mol	Joback Method
log10ws	-8.13		Crippen Method
logp	7.531		Crippen Method
mcvol	369.210	ml/mol	McGowan Method
pc	807.54	kPa	Joback Method
rinpol	2296.00		NIST Webbook
rinpol	2296.00		NIST Webbook
tb	892.01	K	Joback Method
tc	1093.28	K	Joback Method
tf	496.17	K	Joback Method
vc	1.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1239.42	J/mol×K	892.01	Joback Method
cpg	1258.76	J/mol×K	925.56	Joback Method
cpg	1276.83	J/mol×K	959.10	Joback Method
cpg	1293.69	J/mol×K	992.65	Joback Method
cpg	1309.42	J/mol×K	1026.19	Joback Method
cpg	1324.08	J/mol×K	1059.74	Joback Method
cpg	1337.74	J/mol×K	1093.28	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=U370824&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