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

Inchi: InChI=1S/C26H47F3O4/c1-5-8-9-10-11-12-13-14-15-16-17-18-19-20-21-32-23(30)25(6-2
InchiKey: FDRSWKUWSSPWLO-UHFFFAOYSA-N
Formula: C26H47F3O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OC(C)C(F)(F)F
Mol. weight [g/mol]: 480.64

Physical Properties

Property code	Value	Unit	Source
gf	-880.99	kJ/mol	Joback Method
hf	-1680.68	kJ/mol	Joback Method
hfus	59.56	kJ/mol	Joback Method
hvap	86.35	kJ/mol	Joback Method
log10ws	-8.96		Crippen Method
logp	8.311		Crippen Method
mcvol	397.390	ml/mol	McGowan Method
pc	726.14	kPa	Joback Method
rinpol	2502.00		NIST Webbook
rinpol	2502.00		NIST Webbook
tb	937.77	K	Joback Method
tc	1154.61	K	Joback Method
tf	518.71	K	Joback Method
vc	1.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1365.79	J/mol×K	937.77	Joback Method
cpg	1386.43	J/mol×K	973.91	Joback Method
cpg	1405.61	J/mol×K	1010.05	Joback Method
cpg	1423.41	J/mol×K	1046.19	Joback Method
cpg	1439.94	J/mol×K	1082.33	Joback Method
cpg	1455.28	J/mol×K	1118.47	Joback Method
cpg	1469.52	J/mol×K	1154.61	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=U370826&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