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

Inchi: InChI=1S/C27H49F3O4/c1-5-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-33-24(31)26

InchiKey: KJOHBCXCKNVAOR-UHFFFAOYSA-N

Formula: C27H49F3O4

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

Mol. weight [g/mol]: 494.67

Physical Properties

Property code	Value	Unit	Source
gf	-872.57	kJ/mol	Joback Method
hf	-1701.32	kJ/mol	Joback Method
hfus	62.15	kJ/mol	Joback Method
hvap	88.58	kJ/mol	Joback Method
log10ws	-9.38		Crippen Method
logp	8.701		Crippen Method
mcvol	411.480	ml/mol	McGowan Method
pc	689.98	kPa	Joback Method
rinpol	2604.00		NIST Webbook
tb	960.65	K	Joback Method
tc	1187.05	K	Joback Method
tf	529.98	K	Joback Method
vc	1.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1429.73	J/mol×K	960.65	Joback Method
cpg	1451.13	J/mol×K	998.38	Joback Method
cpg	1470.94	J/mol×K	1036.12	Joback Method
cpg	1489.28	J/mol×K	1073.85	Joback Method
cpg	1506.26	J/mol×K	1111.59	Joback Method
cpg	1521.99	J/mol×K	1149.32	Joback Method
cpg	1536.57	J/mol×K	1187.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370827&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

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