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

Inchi: InChI=1S/C25H45F3O4/c1-5-8-9-10-11-12-13-14-15-16-17-18-19-20-31-22(29)24(6-2,7-

InchiKey: CSPGGGMCKKHFKJ-UHFFFAOYSA-N

Formula: C25H45F3O4

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

Mol. weight [g/mol]: 466.62

Physical Properties

Property code	Value	Unit	Source
gf	-889.41	kJ/mol	Joback Method
hf	-1660.04	kJ/mol	Joback Method
hfus	56.97	kJ/mol	Joback Method
hvap	84.12	kJ/mol	Joback Method
log10ws	-8.55		Crippen Method
logp	7.921		Crippen Method
mcvol	383.300	ml/mol	McGowan Method
pc	765.21	kPa	Joback Method
rinpol	2399.00		NIST Webbook
tb	914.89	K	Joback Method
tc	1123.38	K	Joback Method
tf	507.44	K	Joback Method
vc	1.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1302.34	J/mol×K	914.89	Joback Method
cpg	1322.30	J/mol×K	949.64	Joback Method
cpg	1340.89	J/mol×K	984.39	Joback Method
cpg	1358.21	J/mol×K	1019.14	Joback Method
cpg	1374.32	J/mol×K	1053.89	Joback Method
cpg	1389.30	J/mol×K	1088.64	Joback Method
cpg	1403.24	J/mol×K	1123.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370825&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