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

Inchi: InChI=1S/C22H39F3O4/c1-5-8-9-10-11-12-13-14-15-16-17-28-19(26)21(6-2,7-3)20(27)2

InchiKey: TZFVWCWCFBDHKH-UHFFFAOYSA-N

Formula: C22H39F3O4

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

Mol. weight [g/mol]: 424.54

Physical Properties

Property code	Value	Unit	Source
gf	-914.67	kJ/mol	Joback Method
hf	-1598.12	kJ/mol	Joback Method
hfus	49.20	kJ/mol	Joback Method
hvap	77.45	kJ/mol	Joback Method
log10ws	-7.29		Crippen Method
logp	6.751		Crippen Method
mcvol	341.030	ml/mol	McGowan Method
pc	903.43	kPa	Joback Method
rinpol	2096.00		NIST Webbook
tb	846.25	K	Joback Method
tc	1036.12	K	Joback Method
tf	473.63	K	Joback Method
vc	1.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1115.37	J/mol×K	846.25	Joback Method
cpg	1133.65	J/mol×K	877.90	Joback Method
cpg	1150.79	J/mol×K	909.54	Joback Method
cpg	1166.86	J/mol×K	941.19	Joback Method
cpg	1181.91	J/mol×K	972.83	Joback Method
cpg	1195.99	J/mol×K	1004.48	Joback Method
cpg	1209.15	J/mol×K	1036.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370822&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