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

Inchi: InChI=1S/C23H41F3O4/c1-5-8-9-10-11-12-13-14-15-16-17-18-29-20(27)22(6-2,7-3)21(2

InchiKey: BRYLAYHIIFOQIK-UHFFFAOYSA-N

Formula: C23H41F3O4

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

Mol. weight [g/mol]: 438.56

Physical Properties

Property code	Value	Unit	Source
gf	-906.25	kJ/mol	Joback Method
hf	-1618.76	kJ/mol	Joback Method
hfus	51.79	kJ/mol	Joback Method
hvap	79.67	kJ/mol	Joback Method
log10ws	-7.71		Crippen Method
logp	7.141		Crippen Method
mcvol	355.120	ml/mol	McGowan Method
pc	853.47	kPa	Joback Method
rinpol	2194.00		NIST Webbook
tb	869.13	K	Joback Method
tc	1064.22	K	Joback Method
tf	484.90	K	Joback Method
vc	1.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1177.08	J/mol×K	869.13	Joback Method
cpg	1195.86	J/mol×K	901.65	Joback Method
cpg	1213.45	J/mol×K	934.16	Joback Method
cpg	1229.90	J/mol×K	966.68	Joback Method
cpg	1245.27	J/mol×K	999.19	Joback Method
cpg	1259.63	J/mol×K	1031.71	Joback Method
cpg	1273.04	J/mol×K	1064.22	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=U370823&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