Diethylmalonic acid, tridecyl 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C23H39F5O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-31-19(29)21(5-2,6-3)20(30)

InchiKey: AOEJQAHBLQCGPI-UHFFFAOYSA-N

Formula: C23H39F5O4

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

Mol. weight [g/mol]: 474.55

Physical Properties

Property code	Value	Unit	Source
gf	-1290.59	kJ/mol	Joback Method
hf	-2014.45	kJ/mol	Joback Method
hfus	54.06	kJ/mol	Joback Method
hvap	77.13	kJ/mol	Joback Method
log10ws	-7.91		Crippen Method
logp	7.388		Crippen Method
mcvol	358.660	ml/mol	McGowan Method
pc	815.39	kPa	Joback Method
rinpol	2109.00		NIST Webbook
tb	864.88	K	Joback Method
tc	1059.91	K	Joback Method
tf	503.50	K	Joback Method
vc	1.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1191.45	J/mol×K	864.88	Joback Method
cpg	1209.85	J/mol×K	897.38	Joback Method
cpg	1227.09	J/mol×K	929.89	Joback Method
cpg	1243.25	J/mol×K	962.39	Joback Method
cpg	1258.42	J/mol×K	994.90	Joback Method
cpg	1272.67	J/mol×K	1027.40	Joback Method
cpg	1286.07	J/mol×K	1059.91	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=U370850&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