Dimethylmalonic acid, 2,2,3,3,3-pentafluoropropyl tetradecyl ester

Inchi: InChI=1S/C22H37F5O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-30-18(28)20(2,3)19(29)31
InchiKey: VJXNBKIPJUZECP-UHFFFAOYSA-N
Formula: C22H37F5O4
SMILES: CCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCC(F)(F)C(F)(F)F
Mol. weight [g/mol]: 460.52

Physical Properties

Property code	Value	Unit	Source
gf	-1299.01	kJ/mol	Joback Method
hf	-1993.81	kJ/mol	Joback Method
hfus	51.47	kJ/mol	Joback Method
hvap	74.91	kJ/mol	Joback Method
log10ws	-7.49		Crippen Method
logp	6.998		Crippen Method
mcvol	344.570	ml/mol	McGowan Method
pc	862.01	kPa	Joback Method
rinpol	2080.00		NIST Webbook
rinpol	2080.00		NIST Webbook
tb	842.00	K	Joback Method
tc	1030.96	K	Joback Method
tf	492.23	K	Joback Method
vc	1.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1130.15	J/mol×K	842.00	Joback Method
cpg	1147.95	J/mol×K	873.49	Joback Method
cpg	1164.65	J/mol×K	904.99	Joback Method
cpg	1180.33	J/mol×K	936.48	Joback Method
cpg	1195.06	J/mol×K	967.97	Joback Method
cpg	1208.90	J/mol×K	999.47	Joback Method
cpg	1221.92	J/mol×K	1030.96	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=U361947&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