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

Inchi: InChI=1S/C22H38F4O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-29-19(27)21(2,3)20(28)30
InchiKey: BRYGKRVECRFXSW-UHFFFAOYSA-N
Formula: C22H38F4O4
SMILES: CCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCC(F)(F)C(F)F
Mol. weight [g/mol]: 442.53

Physical Properties

Property code	Value	Unit	Source
gf	-1109.48	kJ/mol	Joback Method
hf	-1794.23	kJ/mol	Joback Method
hfus	52.28	kJ/mol	Joback Method
hvap	76.63	kJ/mol	Joback Method
log10ws	-7.14		Crippen Method
logp	6.700		Crippen Method
mcvol	342.800	ml/mol	McGowan Method
pc	879.48	kPa	Joback Method
rinpol	2210.00		NIST Webbook
tb	845.52	K	Joback Method
tc	1035.24	K	Joback Method
tf	474.22	K	Joback Method
vc	1.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1122.65	J/mol×K	845.52	Joback Method
cpg	1140.81	J/mol×K	877.14	Joback Method
cpg	1157.84	J/mol×K	908.76	Joback Method
cpg	1173.79	J/mol×K	940.38	Joback Method
cpg	1188.72	J/mol×K	972.00	Joback Method
cpg	1202.67	J/mol×K	1003.62	Joback Method
cpg	1215.72	J/mol×K	1035.24	Joback Method

Sources

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=U361925&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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