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

Inchi: InChI=1S/C26H46F4O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-33-23(31)25(
InchiKey: IYMAKYJUSAXMKV-UHFFFAOYSA-N
Formula: C26H46F4O4
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCC(F)(F)C(F)F
Mol. weight [g/mol]: 498.63

Physical Properties

Property code	Value	Unit	Source
gf	-1075.80	kJ/mol	Joback Method
hf	-1876.79	kJ/mol	Joback Method
hfus	62.64	kJ/mol	Joback Method
hvap	85.53	kJ/mol	Joback Method
log10ws	-8.82		Crippen Method
logp	8.261		Crippen Method
mcvol	399.160	ml/mol	McGowan Method
pc	708.84	kPa	Joback Method
rinpol	2596.00		NIST Webbook
rinpol	2596.00		NIST Webbook
tb	937.04	K	Joback Method
tc	1157.15	K	Joback Method
tf	519.30	K	Joback Method
vc	1.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1372.69	J/mol×K	937.04	Joback Method
cpg	1393.51	J/mol×K	973.72	Joback Method
cpg	1412.82	J/mol×K	1010.41	Joback Method
cpg	1430.71	J/mol×K	1047.09	Joback Method
cpg	1447.30	J/mol×K	1083.78	Joback Method
cpg	1462.67	J/mol×K	1120.46	Joback Method
cpg	1476.93	J/mol×K	1157.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361928&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

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