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

Inchi: InChI=1S/C19H32F4O4/c1-4-5-6-7-8-9-10-11-12-13-26-16(24)18(2,3)17(25)27-14-19(22

InchiKey: CNCSWFGRVVWCLI-UHFFFAOYSA-N

Formula: C19H32F4O4

SMILES: CCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 400.45

Physical Properties

Property code	Value	Unit	Source
gf	-1134.74	kJ/mol	Joback Method
hf	-1732.31	kJ/mol	Joback Method
hfus	44.51	kJ/mol	Joback Method
hvap	69.95	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	5.530		Crippen Method
mcvol	300.530	ml/mol	McGowan Method
pc	1051.41	kPa	Joback Method
rinpol	1921.00		NIST Webbook
rinpol	1921.00		NIST Webbook
tb	776.88	K	Joback Method
tc	953.87	K	Joback Method
tf	440.41	K	Joback Method
vc	1.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	942.14	J/mol×K	776.88	Joback Method
cpg	958.83	J/mol×K	806.38	Joback Method
cpg	974.56	J/mol×K	835.88	Joback Method
cpg	989.36	J/mol×K	865.37	Joback Method
cpg	1003.29	J/mol×K	894.87	Joback Method
cpg	1016.38	J/mol×K	924.37	Joback Method
cpg	1028.66	J/mol×K	953.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361922&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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