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

Inchi: InChI=1S/C21H36F4O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-28-18(26)20(2,3)19(27)29-16
InchiKey: CHTNJSVWRHOTDT-UHFFFAOYSA-N
Formula: C21H36F4O4
SMILES: CCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCC(F)(F)C(F)F
Mol. weight [g/mol]: 428.50

Physical Properties

Property code	Value	Unit	Source
gf	-1117.90	kJ/mol	Joback Method
hf	-1773.59	kJ/mol	Joback Method
hfus	49.69	kJ/mol	Joback Method
hvap	74.40	kJ/mol	Joback Method
log10ws	-6.72		Crippen Method
logp	6.310		Crippen Method
mcvol	328.710	ml/mol	McGowan Method
pc	931.78	kPa	Joback Method
rinpol	2114.00		NIST Webbook
rinpol	2114.00		NIST Webbook
tb	822.64	K	Joback Method
tc	1007.28	K	Joback Method
tf	462.95	K	Joback Method
vc	1.304	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1061.72	J/mol×K	822.64	Joback Method
cpg	1079.35	J/mol×K	853.41	Joback Method
cpg	1095.92	J/mol×K	884.19	Joback Method
cpg	1111.46	J/mol×K	914.96	Joback Method
cpg	1126.04	J/mol×K	945.74	Joback Method
cpg	1139.70	J/mol×K	976.51	Joback Method
cpg	1152.48	J/mol×K	1007.28	Joback Method

Sources

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=U361924&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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