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

Inchi: InChI=1S/C20H34F4O4/c1-4-5-6-7-8-9-10-11-12-13-14-27-17(25)19(2,3)18(26)28-15-20

InchiKey: ZRZAFVXHJUUEGN-UHFFFAOYSA-N

Formula: C20H34F4O4

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

Mol. weight [g/mol]: 414.48

Physical Properties

Property code	Value	Unit	Source
gf	-1126.32	kJ/mol	Joback Method
hf	-1752.95	kJ/mol	Joback Method
hfus	47.10	kJ/mol	Joback Method
hvap	72.18	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	5.920		Crippen Method
mcvol	314.620	ml/mol	McGowan Method
pc	988.88	kPa	Joback Method
rinpol	2020.00		NIST Webbook
tb	799.76	K	Joback Method
tc	980.18	K	Joback Method
tf	451.68	K	Joback Method
vc	1.248	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1001.53	J/mol×K	799.76	Joback Method
cpg	1018.67	J/mol×K	829.83	Joback Method
cpg	1034.81	J/mol×K	859.90	Joback Method
cpg	1049.98	J/mol×K	889.97	Joback Method
cpg	1064.22	J/mol×K	920.04	Joback Method
cpg	1077.59	J/mol×K	950.11	Joback Method
cpg	1090.12	J/mol×K	980.18	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=U361923&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