

Dimethylmalonic acid, di(2,2,3,3-tetrafluoropropyl) ester

Inchi: InChI=1S/C11H12F8O4/c1-9(2,7(20)22-3-10(16,17)5(12)13)8(21)23-4-11(18,19)6(14)15

InchiKey: NGSRLBYFZNOJAN-UHFFFAOYSA-N

Formula: C11H12F8O4

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

Mol. weight [g/mol]: 360.20

Physical Properties

Property code	Value	Unit	Source
gf	-1980.94	kJ/mol	Joback Method
hf	-2365.66	kJ/mol	Joback Method
hfus	25.17	kJ/mol	Joback Method
hvap	47.19	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.900		Crippen Method
mcvol	194.890	ml/mol	McGowan Method
pc	1640.43	kPa	Joback Method
rinpol	1123.00		NIST Webbook
rinpol	1123.00		NIST Webbook
tb	587.25	K	Joback Method
tc	743.81	K	Joback Method
tf	340.03	K	Joback Method
vc	0.798	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.41	J/mol×K	587.25	Joback Method
cpg	552.40	J/mol×K	613.34	Joback Method
cpg	563.70	J/mol×K	639.44	Joback Method
cpg	574.34	J/mol×K	665.53	Joback Method
cpg	584.35	J/mol×K	691.62	Joback Method
cpg	593.75	J/mol×K	717.72	Joback Method
cpg	602.57	J/mol×K	743.81	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=U361929&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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