

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

Inchi:	InChI=1S/C16H26F4O4/c1-4-5-6-7-8-9-10-23-13(21)15(2,3)14(22)24-11-16(19,20)12(17)
InchiKey:	IQFKPWYFOJSDBT-UHFFFAOYSA-N
Formula:	C16H26F4O4
SMILES:	CCCCCCCCOC(=O)C(C)(C)C(=O)OCC(F)(F)C(F)F
Mol. weight [g/mol]:	358.37

Physical Properties

Property code	Value	Unit	Source
gf	-1160.00	kJ/mol	Joback Method
hf	-1670.39	kJ/mol	Joback Method
hfus	36.74	kJ/mol	Joback Method
hvap	63.27	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.360		Crippen Method
mvol	258.260	ml/mol	McGowan Method
pc	1279.16	kPa	Joback Method
rinpol	1638.00		NIST Webbook
rinpol	1638.00		NIST Webbook
tb	708.24	K	Joback Method
tc	878.99	K	Joback Method
tf	406.60	K	Joback Method
vc	1.024	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.44	J/mol×K	708.24	Joback Method
cpg	784.86	J/mol×K	736.70	Joback Method
cpg	799.45	J/mol×K	765.16	Joback Method
cpg	813.22	J/mol×K	793.62	Joback Method
cpg	826.21	J/mol×K	822.08	Joback Method
cpg	838.45	J/mol×K	850.54	Joback Method
cpg	849.96	J/mol×K	878.99	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U361919&Units=SI

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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