

Diethylmalonic acid, propyl 2,2,3,3-tetrafluoropropyl ester

Inchi:	InChI=1S/C13H20F4O4/c1-4-7-20-10(18)12(5-2,6-3)11(19)21-8-13(16,17)9(14)15/h9H,4
InchiKey:	NPGZXNMHKWXWJV-UHFFFAOYSA-N
Formula:	C13H20F4O4
SMILES:	CCCOC(=O)C(CC)(CC)C(=O)OCC(F)(F)C(F)F
Mol. weight [g/mol]:	316.29

Physical Properties

Property code	Value	Unit	Source
gf	-1185.26	kJ/mol	Joback Method
hf	-1608.47	kJ/mol	Joback Method
hfus	28.97	kJ/mol	Joback Method
hvap	56.60	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.190		Crippen Method
mvol	215.990	ml/mol	McGowan Method
pc	1589.81	kPa	Joback Method
rinpol	1294.00		NIST Webbook
rinpol	1294.00		NIST Webbook
tb	639.60	K	Joback Method
tc	809.01	K	Joback Method
tf	372.79	K	Joback Method
vc	0.856	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.46	J/mol×K	639.60	Joback Method
cpg	620.58	J/mol×K	667.84	Joback Method
cpg	633.96	J/mol×K	696.07	Joback Method
cpg	646.60	J/mol×K	724.31	Joback Method
cpg	658.55	J/mol×K	752.54	Joback Method
cpg	669.81	J/mol×K	780.78	Joback Method
cpg	680.41	J/mol×K	809.01	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=U370830&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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