

Diethylmalonic acid, ethyl pentafluorobenzyl ester

Inchi:	InChI=1S/C16H17F5O4/c1-4-16(5-2,14(22)24-6-3)15(23)25-7-8-9(17)11(19)13(21)12(20)
InchiKey:	IHJXMRKEGKMCMD-UHFFFAOYSA-N
Formula:	C16H17F5O4
SMILES:	CCOC(=O)C(CC)(CC)C(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	368.30

Physical Properties

Property code	Value	Unit	Source
gf	-1290.95	kJ/mol	Joback Method
hf	-1673.29	kJ/mol	Joback Method
hfus	42.85	kJ/mol	Joback Method
hvap	69.73	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	3.795		Crippen Method
mvol	236.270	ml/mol	McGowan Method
pc	1465.73	kPa	Joback Method
rinpol	1622.00		NIST Webbook
rinpol	1622.00		NIST Webbook
tb	762.76	K	Joback Method
tc	947.11	K	Joback Method
tf	508.79	K	Joback Method
vc	0.951	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.54	J/molxK	762.76	Joback Method
cpg	698.11	J/molxK	793.48	Joback Method
cpg	709.91	J/molxK	824.21	Joback Method
cpg	720.94	J/molxK	854.93	Joback Method
cpg	731.22	J/molxK	885.66	Joback Method
cpg	740.74	J/molxK	916.38	Joback Method
cpg	749.51	J/molxK	947.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369987&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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