

Diethylmalonic acid, pentafluorobenzyl propyl ester

Inchi:	InChI=1S/C17H19F5O4/c1-4-7-25-15(23)17(5-2,6-3)16(24)26-8-9-10(18)12(20)14(22)13
InchiKey:	XCNMEECZLNVRAQ-UHFFFAOYSA-N
Formula:	C17H19F5O4
SMILES:	CCCOC(=O)C(CC)(CC)C(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	382.32

Physical Properties

Property code	Value	Unit	Source
gf	-1282.53	kJ/mol	Joback Method
hf	-1693.93	kJ/mol	Joback Method
hfus	45.44	kJ/mol	Joback Method
hvap	71.95	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	4.185		Crippen Method
mcvol	250.360	ml/mol	McGowan Method
pc	1363.65	kPa	Joback Method
rinpol	1709.00		NIST Webbook
rinpol	1709.00		NIST Webbook
tb	785.64	K	Joback Method
tc	971.07	K	Joback Method
tf	520.06	K	Joback Method
vc	1.006	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.90	J/molxK	785.64	Joback Method
cpg	753.91	J/molxK	816.55	Joback Method
cpg	766.10	J/molxK	847.45	Joback Method
cpg	777.47	J/molxK	878.36	Joback Method
cpg	788.04	J/molxK	909.26	Joback Method
cpg	797.81	J/molxK	940.17	Joback Method
cpg	806.79	J/molxK	971.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369988&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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