

Diethylmalonic acid, pentafluorobenzyl pentyl ester

Inchi:	InChI=1S/C19H23F5O4/c1-4-7-8-9-27-17(25)19(5-2,6-3)18(26)28-10-11-12(20)14(22)16
InchiKey:	VLKHRYMKXCVBRU-UHFFFAOYSA-N
Formula:	C19H23F5O4
SMILES:	CCCCCOC(=O)C(CC)(CC)C(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	410.38

Physical Properties

Property code	Value	Unit	Source
gf	-1265.69	kJ/mol	Joback Method
hf	-1735.21	kJ/mol	Joback Method
hfus	50.62	kJ/mol	Joback Method
hvap	76.41	kJ/mol	Joback Method
log10ws	-6.52		Crippen Method
logp	4.965		Crippen Method
mcvol	278.540	ml/mol	McGowan Method
pc	1189.06	kPa	Joback Method
rinpol	1874.00		NIST Webbook
rinpol	1874.00		NIST Webbook
tb	831.40	K	Joback Method
tc	1021.03	K	Joback Method
tf	542.60	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	854.49	J/molxK	831.40	Joback Method
cpg	868.34	J/molxK	863.00	Joback Method
cpg	881.25	J/molxK	894.61	Joback Method
cpg	893.23	J/molxK	926.21	Joback Method
cpg	904.30	J/molxK	957.82	Joback Method
cpg	914.48	J/molxK	989.42	Joback Method
cpg	923.78	J/molxK	1021.03	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369991&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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