Diethylmalonic acid, dipentafluorophenyl ester

Inchi: InChI=1S/C19H10F10O4/c1-3-19(4-2,17(30)32-15-11(26)7(22)5(20)8(23)12(15)27)18(31
InchiKey: IFIFPJPMGPOFLS-UHFFFAOYSA-N
Formula: C19H10F10O4
SMILES: CCC(CC)(C(=O)Oc1c(F)c(F)c(F)c(F)c1F)C(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 492.26

Physical Properties

Property code	Value	Unit	Source
gf	-2175.48	kJ/mol	Joback Method
hf	-2536.58	kJ/mol	Joback Method
hfus	58.12	kJ/mol	Joback Method
hvap	77.91	kJ/mol	Joback Method
log10ws	-8.08		Crippen Method
logp	5.395		Crippen Method
mcvol	263.630	ml/mol	McGowan Method
pc	1214.90	kPa	Joback Method
rinpol	1823.00		NIST Webbook
rinpol	1823.00		NIST Webbook
tb	879.33	K	Joback Method
tc	1076.96	K	Joback Method
tf	634.57	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	787.44	J/mol×K	879.33	Joback Method
cpg	797.38	J/mol×K	912.27	Joback Method
cpg	806.39	J/mol×K	945.21	Joback Method
cpg	814.47	J/mol×K	978.14	Joback Method
cpg	821.61	J/mol×K	1011.08	Joback Method
cpg	827.84	J/mol×K	1044.02	Joback Method
cpg	833.14	J/mol×K	1076.96	Joback Method

Sources

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=U370227&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvap:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume