Diethylmalonic acid, pentafluorophenyl propyl ester

Inchi: InChI=1S/C16H17F5O4/c1-4-7-24-14(22)16(5-2,6-3)15(23)25-13-11(20)9(18)8(17)10(19)

InchiKey: MWXHLBVEWXMFPO-UHFFFAOYSA-N

Formula: C16H17F5O4

SMILES: CCCOC(=O)C(CC)(CC)C(=O)Oc1c(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	-5.41		Crippen Method
logp	4.047		Crippen Method
mcvol	236.270	ml/mol	McGowan Method
pc	1465.73	kPa	Joback Method
rinpol	1637.00		NIST Webbook
rinpol	1637.00		NIST Webbook
tb	762.76	K	Joback Method
tc	947.11	K	Joback Method
tf	508.79	K	Joback Method
vc	0.951	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.54	J/mol×K	762.76	Joback Method
cpg	698.11	J/mol×K	793.48	Joback Method
cpg	709.91	J/mol×K	824.21	Joback Method
cpg	720.94	J/mol×K	854.93	Joback Method
cpg	731.22	J/mol×K	885.66	Joback Method
cpg	740.74	J/mol×K	916.38	Joback Method
cpg	749.51	J/mol×K	947.11	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=U370209&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