Diethylmalonic acid, ethyl pentafluorophenyl ester

Inchi: InChI=1S/C15H15F5O4/c1-4-15(5-2,13(21)23-6-3)14(22)24-12-10(19)8(17)7(16)9(18)11

InchiKey: UJGWZKIAQLEFNB-UHFFFAOYSA-N

Formula: C15H15F5O4

SMILES: CCOC(=O)C(CC)(CC)C(=O)Oc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 354.27

Physical Properties

Property code	Value	Unit	Source
gf	-1299.37	kJ/mol	Joback Method
hf	-1652.65	kJ/mol	Joback Method
hfus	40.26	kJ/mol	Joback Method
hvap	67.50	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	3.657		Crippen Method
mcvol	222.180	ml/mol	McGowan Method
pc	1579.71	kPa	Joback Method
rinpol	1560.00		NIST Webbook
rinpol	1560.00		NIST Webbook
tb	739.88	K	Joback Method
tc	923.75	K	Joback Method
tf	497.52	K	Joback Method
vc	0.894	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.24	J/mol×K	739.88	Joback Method
cpg	643.35	J/mol×K	770.52	Joback Method
cpg	654.73	J/mol×K	801.17	Joback Method
cpg	665.39	J/mol×K	831.81	Joback Method
cpg	675.34	J/mol×K	862.46	Joback Method
cpg	684.57	J/mol×K	893.10	Joback Method
cpg	693.10	J/mol×K	923.75	Joback Method

Sources

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=U370208&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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