Diethylmalonic acid, ethyl 2,2,3,3,4,4,4-heptafluorobutyl ester

Inchi: InChI=1S/C13H17F7O4/c1-4-10(5-2,8(21)23-6-3)9(22)24-7-11(14,15)12(16,17)13(18,19)

InchiKey: WTALSGPMYBXNIS-UHFFFAOYSA-N

Formula: C13H17F7O4

SMILES: CCOC(=O)C(CC)(CC)C(=O)OCC(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 370.26

Physical Properties

Property code	Value	Unit	Source
gf	-1761.57	kJ/mol	Joback Method
hf	-2209.02	kJ/mol	Joback Method
hfus	26.90	kJ/mol	Joback Method
hvap	51.94	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.732		Crippen Method
mcvol	221.300	ml/mol	McGowan Method
pc	1464.61	kPa	Joback Method
rinpol	1216.00		NIST Webbook
rinpol	1216.00		NIST Webbook
tb	631.39	K	Joback Method
tc	795.05	K	Joback Method
tf	394.40	K	Joback Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	635.93	J/mol×K	631.39	Joback Method
cpg	649.25	J/mol×K	658.67	Joback Method
cpg	661.76	J/mol×K	685.94	Joback Method
cpg	673.48	J/mol×K	713.22	Joback Method
cpg	684.48	J/mol×K	740.49	Joback Method
cpg	694.78	J/mol×K	767.77	Joback Method
cpg	704.44	J/mol×K	795.05	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=U368426&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