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

Inchi: InChI=1S/C15H21F7O4/c1-5-12(6-2,10(23)25-7-9(3)4)11(24)26-8-13(16,17)14(18,19)15(

InchiKey: FFEPQNSOTYUWMM-UHFFFAOYSA-N

Formula: C15H21F7O4

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

Mol. weight [g/mol]: 398.31

Physical Properties

Property code	Value	Unit	Source
gf	-1747.17	kJ/mol	Joback Method
hf	-2255.58	kJ/mol	Joback Method
hfus	28.56	kJ/mol	Joback Method
hvap	56.00	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.368		Crippen Method
mcvol	249.480	ml/mol	McGowan Method
pc	1278.25	kPa	Joback Method
rinpol	1337.00		NIST Webbook
rinpol	1337.00		NIST Webbook
tb	676.71	K	Joback Method
tc	843.35	K	Joback Method
tf	401.94	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	742.62	J/mol×K	676.71	Joback Method
cpg	756.89	J/mol×K	704.48	Joback Method
cpg	770.29	J/mol×K	732.26	Joback Method
cpg	782.87	J/mol×K	760.03	Joback Method
cpg	794.66	J/mol×K	787.80	Joback Method
cpg	805.73	J/mol×K	815.58	Joback Method
cpg	816.11	J/mol×K	843.35	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=U368428&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