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

Inchi: InChI=1S/C14H19F7O4/c1-4-7-24-9(22)11(5-2,6-3)10(23)25-8-12(15,16)13(17,18)14(19,

InchiKey: JTQWDBBWAQXEMN-UHFFFAOYSA-N

Formula: C14H19F7O4

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

Mol. weight [g/mol]: 384.29

Physical Properties

Property code	Value	Unit	Source
gf	-1753.15	kJ/mol	Joback Method
hf	-2229.66	kJ/mol	Joback Method
hfus	29.49	kJ/mol	Joback Method
hvap	54.17	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	4.122		Crippen Method
mcvol	235.390	ml/mol	McGowan Method
pc	1362.64	kPa	Joback Method
rinpol	1294.00		NIST Webbook
rinpol	1294.00		NIST Webbook
tb	654.27	K	Joback Method
tc	818.36	K	Joback Method
tf	405.67	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.45	J/mol×K	654.27	Joback Method
cpg	702.17	J/mol×K	681.62	Joback Method
cpg	715.05	J/mol×K	708.97	Joback Method
cpg	727.14	J/mol×K	736.32	Joback Method
cpg	738.49	J/mol×K	763.66	Joback Method
cpg	749.14	J/mol×K	791.01	Joback Method
cpg	759.13	J/mol×K	818.36	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=U368427&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