Diethylmalonic acid, di(2,2,3,3,4,4,4-heptafluorobutyl) ester

Inchi: InChI=1S/C15H14F14O4/c1-3-9(4-2,7(30)32-5-10(16,17)12(20,21)14(24,25)26)8(31)33-6
InchiKey: DLZONRAVRLWNTL-UHFFFAOYSA-N
Formula: C15H14F14O4
SMILES: CCC(CC)(C(=O)OCC(F)(F)C(F)(F)C(F)(F)F)C(=O)OCC(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 524.25

Physical Properties

Property code	Value	Unit	Source
gf	-3099.88	kJ/mol	Joback Method
hf	-3649.32	kJ/mol	Joback Method
hfus	31.40	kJ/mol	Joback Method
hvap	46.79	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.545		Crippen Method
mcvol	261.870	ml/mol	McGowan Method
pc	1065.87	kPa	Joback Method
rinpol	1155.00		NIST Webbook
tb	662.35	K	Joback Method
tc	815.36	K	Joback Method
tf	428.33	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	805.68	J/mol×K	662.35	Joback Method
cpg	818.14	J/mol×K	687.85	Joback Method
cpg	829.72	J/mol×K	713.35	Joback Method
cpg	840.47	J/mol×K	738.85	Joback Method
cpg	850.45	J/mol×K	764.35	Joback Method
cpg	859.73	J/mol×K	789.86	Joback Method
cpg	868.37	J/mol×K	815.36	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=U368444&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