Diethylmalonic acid, di(2,2,3,3,4,4,5,5-octafluoropentyl) ester

Inchi: InChI=1S/C17H16F16O4/c1-3-11(4-2,9(34)36-5-12(22,23)16(30,31)14(26,27)7(18)19)10
InchiKey: UARSSTLFGUXQGB-UHFFFAOYSA-N
Formula: C17H16F16O4
SMILES: CCC(CC)(C(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)F)C(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F
Mol. weight [g/mol]: 588.28

Physical Properties

Property code	Value	Unit	Source
gf	-3477.54	kJ/mol	Joback Method
hf	-4093.38	kJ/mol	Joback Method
hfus	35.70	kJ/mol	Joback Method
hvap	48.83	kJ/mol	Joback Method
log10ws	-6.93		Crippen Method
logp	6.221		Crippen Method
mcvol	293.590	ml/mol	McGowan Method
pc	902.34	kPa	Joback Method
rinpol	1395.00		NIST Webbook
rinpol	1395.00		NIST Webbook
tb	705.77	K	Joback Method
tc	864.21	K	Joback Method
tf	422.05	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	930.68	J/mol×K	705.77	Joback Method
cpg	943.77	J/mol×K	732.18	Joback Method
cpg	955.91	J/mol×K	758.58	Joback Method
cpg	967.20	J/mol×K	784.99	Joback Method
cpg	977.68	J/mol×K	811.40	Joback Method
cpg	987.45	J/mol×K	837.80	Joback Method
cpg	996.56	J/mol×K	864.21	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U370668&Units=SI

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