Diethylmalonic acid, 2-methylhex-3-yl 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C17H27F5O4/c1-6-9-12(11(4)5)26-14(24)15(7-2,8-3)13(23)25-10-16(18,19)17

InchiKey: XBLUODVGWMIYKE-UHFFFAOYSA-N

Formula: C17H27F5O4

SMILES: CCCC(OC(=O)C(CC)(CC)C(=O)OCC(F)(F)C(F)(F)F)C(C)C

Mol. weight [g/mol]: 390.39

Physical Properties

Property code	Value	Unit	Source
gf	-1345.99	kJ/mol	Joback Method
hf	-1901.17	kJ/mol	Joback Method
hfus	31.47	kJ/mol	Joback Method
hvap	63.00	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.901		Crippen Method
mcvol	274.120	ml/mol	McGowan Method
pc	1180.90	kPa	Joback Method
rinpol	1431.00		NIST Webbook
tb	726.72	K	Joback Method
tc	900.63	K	Joback Method
tf	405.88	K	Joback Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	836.24	J/mol×K	726.72	Joback Method
cpg	851.98	J/mol×K	755.70	Joback Method
cpg	866.79	J/mol×K	784.69	Joback Method
cpg	880.73	J/mol×K	813.67	Joback Method
cpg	893.82	J/mol×K	842.66	Joback Method
cpg	906.13	J/mol×K	871.64	Joback Method
cpg	917.68	J/mol×K	900.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370842&Units=SI
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

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