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

Inchi: InChI=1S/C17H25F7O4/c1-4-7-8-9-10-27-12(25)14(5-2,6-3)13(26)28-11-15(18,19)16(20

InchiKey: YFFDZADHXZSOEL-UHFFFAOYSA-N

Formula: C17H25F7O4

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

Mol. weight [g/mol]: 426.37

Physical Properties

Property code	Value	Unit	Source
gf	-1727.89	kJ/mol	Joback Method
hf	-2291.58	kJ/mol	Joback Method
hfus	37.26	kJ/mol	Joback Method
hvap	60.84	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	5.292		Crippen Method
mcvol	277.660	ml/mol	McGowan Method
pc	1113.34	kPa	Joback Method
rinpol	1543.00		NIST Webbook
rinpol	1543.00		NIST Webbook
tb	722.91	K	Joback Method
tc	891.17	K	Joback Method
tf	439.48	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	852.81	J/mol×K	722.91	Joback Method
cpg	867.68	J/mol×K	750.95	Joback Method
cpg	881.67	J/mol×K	779.00	Joback Method
cpg	894.82	J/mol×K	807.04	Joback Method
cpg	907.18	J/mol×K	835.08	Joback Method
cpg	918.82	J/mol×K	863.12	Joback Method
cpg	929.77	J/mol×K	891.17	Joback Method

Sources

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=U368431&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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