Diethylmalonic acid, 2,2,3,3,3-pentafluoropropyl octyl ester

Inchi: InChI=1S/C18H29F5O4/c1-4-7-8-9-10-11-12-26-14(24)16(5-2,6-3)15(25)27-13-17(19,20)18(21,22)23

InchiKey: JZZGUSXKLJMZGZ-UHFFFAOYSA-N

Formula: C18H29F5O4

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

Mol. weight [g/mol]: 404.41

Physical Properties

Property code	Value	Unit	Source
gf	-1332.69	kJ/mol	Joback Method
hf	-1911.25	kJ/mol	Joback Method
hfus	41.11	kJ/mol	Joback Method
hvap	66.00	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	5.437		Crippen Method
mcvol	288.210	ml/mol	McGowan Method
pc	1094.99	kPa	Joback Method
rinpol	1621.00		NIST Webbook
rinpol	1621.00		NIST Webbook
tb	750.48	K	Joback Method
tc	923.72	K	Joback Method
tf	447.15	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	892.50	J/mol×K	750.48	Joback Method
cpg	908.35	J/mol×K	779.35	Joback Method
cpg	923.30	J/mol×K	808.23	Joback Method
cpg	937.38	J/mol×K	837.10	Joback Method
cpg	950.63	J/mol×K	865.98	Joback Method
cpg	963.12	J/mol×K	894.85	Joback Method
cpg	974.87	J/mol×K	923.72	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=U370845&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