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

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

InchiKey: LDCWGWQLXMGCRS-UHFFFAOYSA-N

Formula: C17H27F5O4

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

Mol. weight [g/mol]: 390.39

Physical Properties

Property code	Value	Unit	Source
gf	-1341.11	kJ/mol	Joback Method
hf	-1890.61	kJ/mol	Joback Method
hfus	38.52	kJ/mol	Joback Method
hvap	63.78	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	5.047		Crippen Method
mcvol	274.120	ml/mol	McGowan Method
pc	1168.02	kPa	Joback Method
rinpol	1541.00		NIST Webbook
rinpol	1541.00		NIST Webbook
tb	727.60	K	Joback Method
tc	898.72	K	Joback Method
tf	435.88	K	Joback Method
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	835.25	J/mol×K	727.60	Joback Method
cpg	850.70	J/mol×K	756.12	Joback Method
cpg	865.27	J/mol×K	784.64	Joback Method
cpg	878.99	J/mol×K	813.16	Joback Method
cpg	891.92	J/mol×K	841.68	Joback Method
cpg	904.10	J/mol×K	870.20	Joback Method
cpg	915.56	J/mol×K	898.72	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=U370844&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