Diethylmalonic acid, heptadecyl pentafluorophenyl ester

Inchi: InChI=1S/C30H45F5O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-38-28(36)30(5

InchiKey: HBNJUCXBGPQKHA-UHFFFAOYSA-N

Formula: C30H45F5O4

SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 564.67

Physical Properties

Property code	Value	Unit	Source
gf	-1173.07	kJ/mol	Joback Method
hf	-1962.25	kJ/mol	Joback Method
hfus	79.11	kJ/mol	Joback Method
hvap	100.89	kJ/mol	Joback Method
log10ws	-11.27		Crippen Method
logp	9.509		Crippen Method
mcvol	433.530	ml/mol	McGowan Method
pc	638.98	kPa	Joback Method
rinpol	2998.00		NIST Webbook
tb	1083.08	K	Joback Method
tc	1367.58	K	Joback Method
tf	666.57	K	Joback Method
vc	1.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1525.73	J/mol×K	1083.08	Joback Method
cpg	1545.18	J/mol×K	1130.50	Joback Method
cpg	1562.14	J/mol×K	1177.91	Joback Method
cpg	1576.74	J/mol×K	1225.33	Joback Method
cpg	1589.11	J/mol×K	1272.75	Joback Method
cpg	1599.41	J/mol×K	1320.16	Joback Method
cpg	1607.77	J/mol×K	1367.58	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=U370224&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

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