Diethylmalonic acid, octadecyl pentafluorobenzyl ester

Inchi: InChI=1S/C32H49F5O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-40-30(38)3

InchiKey: WXNCOZHSLFVTPI-UHFFFAOYSA-N

Formula: C32H49F5O4

SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 592.72

Physical Properties

Property code	Value	Unit	Source
gf	-1156.23	kJ/mol	Joback Method
hf	-2003.53	kJ/mol	Joback Method
hfus	84.29	kJ/mol	Joback Method
hvap	105.34	kJ/mol	Joback Method
log10ws	-11.96		Crippen Method
logp	10.036		Crippen Method
mcvol	461.710	ml/mol	McGowan Method
pc	581.20	kPa	Joback Method
rinpol	3156.00		NIST Webbook
rinpol	3156.00		NIST Webbook
tb	1128.84	K	Joback Method
tc	1449.79	K	Joback Method
tf	689.11	K	Joback Method
vc	1.847	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1652.80	J/mol×K	1128.84	Joback Method
cpg	1673.66	J/mol×K	1182.33	Joback Method
cpg	1691.40	J/mol×K	1235.82	Joback Method
cpg	1706.24	J/mol×K	1289.31	Joback Method
cpg	1718.40	J/mol×K	1342.80	Joback Method
cpg	1728.10	J/mol×K	1396.30	Joback Method
cpg	1735.57	J/mol×K	1449.79	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=U370004&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