Diethylmalonic acid, eicosyl pentafluorobenzyl ester

Inchi: InChI=1S/C34H53F5O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-42-3

InchiKey: AMDKEMPLTLFFGX-UHFFFAOYSA-N

Formula: C34H53F5O4

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

Mol. weight [g/mol]: 620.77

Physical Properties

Property code	Value	Unit	Source
gf	-1139.39	kJ/mol	Joback Method
hf	-2044.81	kJ/mol	Joback Method
hfus	89.47	kJ/mol	Joback Method
hvap	109.80	kJ/mol	Joback Method
log10ws	-12.79		Crippen Method
logp	10.817		Crippen Method
mcvol	489.890	ml/mol	McGowan Method
pc	530.91	kPa	Joback Method
rinpol	3354.00		NIST Webbook
tb	1174.60	K	Joback Method
tc	1540.61	K	Joback Method
tf	711.65	K	Joback Method
vc	1.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1780.66	J/mol×K	1174.60	Joback Method
cpg	1803.07	J/mol×K	1235.60	Joback Method
cpg	1821.56	J/mol×K	1296.60	Joback Method
cpg	1836.47	J/mol×K	1357.61	Joback Method
cpg	1848.18	J/mol×K	1418.61	Joback Method
cpg	1857.06	J/mol×K	1479.61	Joback Method
cpg	1863.46	J/mol×K	1540.61	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=U370005&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