Diethylmalonic acid, 2,2,3,3,4,4,5,5-octafluoropentyl tridecyl ester

Inchi: InChI=1S/C25H40F8O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-36-20(34)22(5-2,6-3)21(35

InchiKey: YRGLHLJSTSMQQS-UHFFFAOYSA-N

Formula: C25H40F8O4

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

Mol. weight [g/mol]: 556.57

Physical Properties

Property code	Value	Unit	Source
gf	-1857.78	kJ/mol	Joback Method
hf	-2658.09	kJ/mol	Joback Method
hfus	57.54	kJ/mol	Joback Method
hvap	77.45	kJ/mol	Joback Method
log10ws	-9.03		Crippen Method
logp	8.361		Crippen Method
mcvol	392.150	ml/mol	McGowan Method
pc	691.79	kPa	Joback Method
rinpol	2306.00		NIST Webbook
tb	904.78	K	Joback Method
tc	1117.57	K	Joback Method
tf	515.23	K	Joback Method
vc	1.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1337.62	J/mol×K	904.78	Joback Method
cpg	1357.12	J/mol×K	940.24	Joback Method
cpg	1375.32	J/mol×K	975.71	Joback Method
cpg	1392.37	J/mol×K	1011.17	Joback Method
cpg	1408.38	J/mol×K	1046.64	Joback Method
cpg	1423.48	J/mol×K	1082.10	Joback Method
cpg	1437.82	J/mol×K	1117.57	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=U370661&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