Diethylmalonic acid, 2,2,3,3,4,4,4-heptafluorobutyl pentadecyl ester

Inchi: InChI=1S/C26H43F7O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-36-21(34)23(5-2,6-3

InchiKey: QUGIRALGMXDFMC-UHFFFAOYSA-N

Formula: C26H43F7O4

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

Mol. weight [g/mol]: 552.61

Physical Properties

Property code	Value	Unit	Source
gf	-1652.11	kJ/mol	Joback Method
hf	-2477.34	kJ/mol	Joback Method
hfus	60.57	kJ/mol	Joback Method
hvap	80.88	kJ/mol	Joback Method
log10ws	-9.48		Crippen Method
logp	8.803		Crippen Method
mcvol	404.470	ml/mol	McGowan Method
pc	670.81	kPa	Joback Method
rinpol	2384.00		NIST Webbook
rinpol	2384.00		NIST Webbook
tb	928.83	K	Joback Method
tc	1149.91	K	Joback Method
tf	540.91	K	Joback Method
vc	1.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1392.90	J/mol×K	928.83	Joback Method
cpg	1413.30	J/mol×K	965.68	Joback Method
cpg	1432.36	J/mol×K	1002.52	Joback Method
cpg	1450.24	J/mol×K	1039.37	Joback Method
cpg	1467.08	J/mol×K	1076.22	Joback Method
cpg	1483.02	J/mol×K	1113.06	Joback Method
cpg	1498.23	J/mol×K	1149.91	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U368440&Units=SI

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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