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

Inchi: InChI=1S/C29H48F8O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-40-24(38)26(5

InchiKey: CLDKJRIXJSOQKG-UHFFFAOYSA-N

Formula: C29H48F8O4

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

Mol. weight [g/mol]: 612.68

Physical Properties

Property code	Value	Unit	Source
gf	-1824.10	kJ/mol	Joback Method
hf	-2740.65	kJ/mol	Joback Method
hfus	67.90	kJ/mol	Joback Method
hvap	86.35	kJ/mol	Joback Method
log10ws	-10.70		Crippen Method
logp	9.922		Crippen Method
mcvol	448.510	ml/mol	McGowan Method
pc	570.69	kPa	Joback Method
rinpol	2680.00		NIST Webbook
rinpol	2680.00		NIST Webbook
tb	996.30	K	Joback Method
tc	1259.47	K	Joback Method
tf	560.31	K	Joback Method
vc	1.802	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1591.39	J/mol×K	996.30	Joback Method
cpg	1615.29	J/mol×K	1040.16	Joback Method
cpg	1637.50	J/mol×K	1084.02	Joback Method
cpg	1658.31	J/mol×K	1127.89	Joback Method
cpg	1677.99	J/mol×K	1171.75	Joback Method
cpg	1696.79	J/mol×K	1215.61	Joback Method
cpg	1715.01	J/mol×K	1259.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370665&Units=SI
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

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