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

Inchi: InChI=1S/C29H49F7O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-39-24(37)2

InchiKey: ONVSTCBOQNRXCW-UHFFFAOYSA-N

Formula: C29H49F7O4

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

Mol. weight [g/mol]: 594.69

Physical Properties

Property code	Value	Unit	Source
gf	-1626.85	kJ/mol	Joback Method
hf	-2539.26	kJ/mol	Joback Method
hfus	68.34	kJ/mol	Joback Method
hvap	87.56	kJ/mol	Joback Method
log10ws	-10.74		Crippen Method
logp	9.974		Crippen Method
mcvol	446.740	ml/mol	McGowan Method
pc	580.92	kPa	Joback Method
rinpol	2673.00		NIST Webbook
rinpol	2673.00		NIST Webbook
tb	997.47	K	Joback Method
tc	1256.68	K	Joback Method
tf	574.72	K	Joback Method
vc	1.790	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1584.43	J/mol×K	997.47	Joback Method
cpg	1608.21	J/mol×K	1040.67	Joback Method
cpg	1630.37	J/mol×K	1083.87	Joback Method
cpg	1651.18	J/mol×K	1127.08	Joback Method
cpg	1670.89	J/mol×K	1170.28	Joback Method
cpg	1689.76	J/mol×K	1213.48	Joback Method
cpg	1708.05	J/mol×K	1256.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368443&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

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