Diethylmalonic acid, hexadecyl 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C26H45F5O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-34-22(32)24(5-2,
InchiKey: FWVAASZGORSNLU-UHFFFAOYSA-N
Formula: C26H45F5O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(F)(F)C(F)(F)F
Mol. weight [g/mol]: 516.63

Physical Properties

Property code	Value	Unit	Source
gf	-1265.33	kJ/mol	Joback Method
hf	-2076.37	kJ/mol	Joback Method
hfus	61.83	kJ/mol	Joback Method
hvap	83.81	kJ/mol	Joback Method
log10ws	-9.17		Crippen Method
logp	8.558		Crippen Method
mcvol	400.930	ml/mol	McGowan Method
pc	696.18	kPa	Joback Method
rinpol	2400.00		NIST Webbook
rinpol	2400.00		NIST Webbook
tb	933.52	K	Joback Method
tc	1153.14	K	Joback Method
tf	537.31	K	Joback Method
vc	1.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1379.09	J/mol×K	933.52	Joback Method
cpg	1399.71	J/mol×K	970.12	Joback Method
cpg	1418.92	J/mol×K	1006.73	Joback Method
cpg	1436.85	J/mol×K	1043.33	Joback Method
cpg	1453.63	J/mol×K	1079.93	Joback Method
cpg	1469.36	J/mol×K	1116.54	Joback Method
cpg	1484.19	J/mol×K	1153.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370853&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