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

Inchi: InChI=1S/C23H37F7O4/c1-4-7-8-9-10-11-12-13-14-15-16-33-18(31)20(5-2,6-3)19(32)34
InchiKey: KETIWCSONQLCTI-UHFFFAOYSA-N
Formula: C23H37F7O4
SMILES: CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 510.53

Physical Properties

Property code	Value	Unit	Source
gf	-1677.37	kJ/mol	Joback Method
hf	-2415.42	kJ/mol	Joback Method
hfus	52.80	kJ/mol	Joback Method
hvap	74.20	kJ/mol	Joback Method
log10ws	-8.22		Crippen Method
logp	7.633		Crippen Method
mcvol	362.200	ml/mol	McGowan Method
pc	783.31	kPa	Joback Method
rinpol	2098.00		NIST Webbook
rinpol	2098.00		NIST Webbook
tb	860.19	K	Joback Method
tc	1055.03	K	Joback Method
tf	507.10	K	Joback Method
vc	1.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1206.42	J/mol×K	860.19	Joback Method
cpg	1224.40	J/mol×K	892.66	Joback Method
cpg	1241.25	J/mol×K	925.14	Joback Method
cpg	1257.07	J/mol×K	957.61	Joback Method
cpg	1271.95	J/mol×K	990.08	Joback Method
cpg	1285.99	J/mol×K	1022.56	Joback Method
cpg	1299.29	J/mol×K	1055.03	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=U368437&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