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

Inchi: InChI=1S/C24H39F7O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-34-19(32)21(5-2,6-3)20(33

InchiKey: NWACKQSTOMJYIF-UHFFFAOYSA-N

Formula: C24H39F7O4

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

Mol. weight [g/mol]: 524.55

Physical Properties

Property code	Value	Unit	Source
gf	-1668.95	kJ/mol	Joback Method
hf	-2436.06	kJ/mol	Joback Method
hfus	55.39	kJ/mol	Joback Method
hvap	76.43	kJ/mol	Joback Method
log10ws	-8.64		Crippen Method
logp	8.023		Crippen Method
mcvol	376.290	ml/mol	McGowan Method
pc	742.86	kPa	Joback Method
rinpol	2197.00		NIST Webbook
rinpol	2197.00		NIST Webbook
tb	883.07	K	Joback Method
tc	1085.50	K	Joback Method
tf	518.37	K	Joback Method
vc	1.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1267.96	J/mol×K	883.07	Joback Method
cpg	1286.66	J/mol×K	916.81	Joback Method
cpg	1304.17	J/mol×K	950.55	Joback Method
cpg	1320.60	J/mol×K	984.29	Joback Method
cpg	1336.06	J/mol×K	1018.03	Joback Method
cpg	1350.66	J/mol×K	1051.77	Joback Method
cpg	1364.51	J/mol×K	1085.50	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=U368438&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