Dimethylmalonic acid, heptadecyl 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C25H43F5O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-33-21(31)23(2,3
InchiKey: CJKDHDFVEAGYEU-UHFFFAOYSA-N
Formula: C25H43F5O4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCC(F)(F)C(F)(F)F
Mol. weight [g/mol]: 502.60

Physical Properties

Property code	Value	Unit	Source
gf	-1273.75	kJ/mol	Joback Method
hf	-2055.73	kJ/mol	Joback Method
hfus	59.24	kJ/mol	Joback Method
hvap	81.58	kJ/mol	Joback Method
log10ws	-8.75		Crippen Method
logp	8.168		Crippen Method
mcvol	386.840	ml/mol	McGowan Method
pc	732.84	kPa	Joback Method
rinpol	2363.00		NIST Webbook
rinpol	2363.00		NIST Webbook
tb	910.64	K	Joback Method
tc	1120.91	K	Joback Method
tf	526.04	K	Joback Method
vc	1.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1315.97	J/mol×K	910.64	Joback Method
cpg	1335.76	J/mol×K	945.69	Joback Method
cpg	1354.25	J/mol×K	980.73	Joback Method
cpg	1371.53	J/mol×K	1015.78	Joback Method
cpg	1387.72	J/mol×K	1050.82	Joback Method
cpg	1402.90	J/mol×K	1085.87	Joback Method
cpg	1417.20	J/mol×K	1120.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361949&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