Diethylmalonic acid, di(2-(3,3-dimethyl-2,4-oxacyclopentyl)ethyl) ester

Inchi: InChI=1S/C21H36O8/c1-7-21(8-2,17(22)24-11-9-15-13-26-19(3,4)28-15)18(23)25-12-10-
InchiKey: IYKBQWFRUJKQLI-UHFFFAOYSA-N
Formula: C21H36O8
SMILES: CCC(CC)(C(=O)OCCC1COC(C)(C)O1)C(=O)OCCC1COC(C)(C)O1
Mol. weight [g/mol]: 416.51

Physical Properties

Property code	Value	Unit	Source
gf	-636.84	kJ/mol	Joback Method
hf	-1392.36	kJ/mol	Joback Method
hfus	57.64	kJ/mol	Joback Method
hvap	94.99	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	2.962		Crippen Method
mcvol	323.390	ml/mol	McGowan Method
pc	1298.60	kPa	Joback Method
rinpol	2384.00		NIST Webbook
tb	958.73	K	Joback Method
tc	1182.16	K	Joback Method
tf	640.57	K	Joback Method
vc	1.208	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1164.99	J/mol×K	958.73	Joback Method
cpg	1189.25	J/mol×K	995.97	Joback Method
cpg	1213.82	J/mol×K	1033.21	Joback Method
cpg	1238.91	J/mol×K	1070.44	Joback Method
cpg	1264.78	J/mol×K	1107.68	Joback Method
cpg	1291.65	J/mol×K	1144.92	Joback Method
cpg	1319.77	J/mol×K	1182.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368392&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