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

Inchi: InChI=1S/C16H28O6/c1-6-16(7-2,13(17)19-8-3)14(18)20-10-9-12-11-21-15(4,5)22-12/h1
InchiKey: DSEMECMSXHKNGY-UHFFFAOYSA-N
Formula: C16H28O6
SMILES: CCOC(=O)C(CC)(CC)C(=O)OCCC1COC(C)(C)O1
Mol. weight [g/mol]: 316.39

Physical Properties

Property code	Value	Unit	Source
gf	-530.05	kJ/mol	Joback Method
hf	-1080.54	kJ/mol	Joback Method
hfus	40.02	kJ/mol	Joback Method
hvap	76.04	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.441		Crippen Method
mcvol	252.060	ml/mol	McGowan Method
pc	1640.43	kPa	Joback Method
rinpol	1831.00		NIST Webbook
tb	779.58	K	Joback Method
tc	983.43	K	Joback Method
tf	500.52	K	Joback Method
vc	0.949	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.41	J/mol×K	779.58	Joback Method
cpg	811.11	J/mol×K	813.55	Joback Method
cpg	828.07	J/mol×K	847.53	Joback Method
cpg	844.38	J/mol×K	881.50	Joback Method
cpg	860.14	J/mol×K	915.48	Joback Method
cpg	875.46	J/mol×K	949.45	Joback Method
cpg	890.42	J/mol×K	983.43	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=U368391&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