Cyclobutane, 1,3-bis[2-(2-isopropyl-3,3-dimethyloxiran-2-yl)ethe

Inchi: InChI=1S/C26H40O4/c1-15(2)25(23(7,8)29-25)13-11-19-21(17(5)27)20(22(19)18(6)28)1

InchiKey: LPGSGNDUSMQLHZ-PHEQNACWSA-N

Formula: C26H40O4

SMILES: CC(=O)C1C(C=CC2(C(C)C)OC2(C)C)C(C(C)=O)C1C=CC1(C(C)C)OC1(C)C

Mol. weight [g/mol]: 416.59

CAS: 70373-02-3

Physical Properties

Property code	Value	Unit	Source
gf	3.16	kJ/mol	Joback Method
hf	-673.75	kJ/mol	Joback Method
hfus	48.08	kJ/mol	Joback Method
hvap	88.88	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	5.162		Crippen Method
mcvol	350.900	ml/mol	McGowan Method
pc	1070.76	kPa	Joback Method
rinpol	2674.00		NIST Webbook
rinpol	2674.00		NIST Webbook
rinpol	2674.00		NIST Webbook
tb	965.46	K	Joback Method
tc	1195.45	K	Joback Method
tf	620.32	K	Joback Method
vc	1.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1286.75	J/mol×K	965.46	Joback Method
cpg	1325.23	J/mol×K	1003.79	Joback Method
cpg	1366.88	J/mol×K	1042.12	Joback Method
cpg	1412.26	J/mol×K	1080.46	Joback Method
cpg	1461.94	J/mol×K	1118.79	Joback Method
cpg	1516.50	J/mol×K	1157.12	Joback Method

cpg	1576.49	J/mol×K	1195.45	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=C70373023&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