

1,3,5-Cyclohexanetriol, 2,2,4,4,6,6-hexamethyl-, triisobutyrate

Inchi:	InChI=1S/C24H42O6/c1-13(2)16(25)28-19-22(7,8)20(29-17(26)14(3)4)24(11,12)21(23(1
InchiKey:	UQSQGZQFVQERPO-UHFFFAOYSA-N
Formula:	C24H42O6
SMILES:	CC(C)C(=O)OC1C(C)(C)C(OC(=O)C(C)C)C(C)(C)C(OC(=O)C(C)C)C1(C)C
Mol. weight [g/mol]:	426.59
CAS:	101611-75-0

Physical Properties

Property code	Value	Unit	Source
gf	-588.45	kJ/mol	Joback Method
hf	-1290.59	kJ/mol	Joback Method
hfus	34.00	kJ/mol	Joback Method
hvap	90.75	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.782		Crippen Method
mcvol	360.480	ml/mol	McGowan Method
pc	985.78	kPa	Joback Method
tb	972.99	K	Joback Method
tc	1194.94	K	Joback Method
tf	589.60	K	Joback Method
vc	1.355	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1300.12	J/molxK	972.99	Joback Method
cpg	1330.22	J/molxK	1009.98	Joback Method
cpg	1361.02	J/molxK	1046.97	Joback Method
cpg	1392.76	J/molxK	1083.97	Joback Method
cpg	1425.71	J/molxK	1120.96	Joback Method
cpg	1460.12	J/molxK	1157.95	Joback Method
cpg	1496.26	J/molxK	1194.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C101611750&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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