Acetal of cyclododecanone and 2,2-dimethyl-1,3-propanediol

Inchi: InChI=1S/C16H32O2/c1-3-17-16(18-4-2)14-12-10-8-6-5-7-9-11-13-15-16/h3-15H2,1-2H3

InchiKey: XMQLLEROFXPBDO-UHFFFAOYSA-N

Formula: C16H32O2

SMILES: CCOC1(OCC)CCCCCCCCCCC1

Mol. weight [g/mol]: 256.42

Physical Properties

Property code	Value	Unit	Source
gf	-179.80	kJ/mol	Joback Method
hf	-605.41	kJ/mol	Joback Method
hfus	12.51	kJ/mol	Joback Method
hvap	56.34	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	5.060		Crippen Method
mcvol	237.180	ml/mol	McGowan Method
pc	1753.60	kPa	Joback Method
rinpol	1908.40		NIST Webbook
rinpol	1930.30		NIST Webbook
rinpol	1896.00		NIST Webbook
ripol	2307.90		NIST Webbook
ripol	2276.80		NIST Webbook
ripol	2237.90		NIST Webbook
tb	655.73	K	Joback Method
tc	880.64	K	Joback Method
tf	324.70	K	Joback Method
vc	0.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	686.14	J/mol×K	655.73	Joback Method
cpg	713.47	J/mol×K	693.21	Joback Method
cpg	739.26	J/mol×K	730.70	Joback Method
cpg	763.57	J/mol×K	768.18	Joback Method

cpg	786.47	J/mol×K	805.67	Joback Method
cpg	808.01	J/mol×K	843.15	Joback Method
cpg	828.26	J/mol×K	880.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R235737&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume