

Isobornyl laureate

Inchi:
InchiKey:
Formula:
SMILES:
Mol. weight [g/mol]:

InChI=1S/C22H40O2/c1-5-6-7-8-9-10-11-12-13-14-20(23)24-19-17-18-15-16-22(19,4)21
SABGETNXHUZLDJ-UHFFFAOYSA-N
C22H40O2
CCCCCCCCCCCC(=O)OC1CC2CCC1(C)C2(C)C
336.55

Physical Properties

Property code	Value	Unit	Source
gf	-16.56	kJ/mol	Joback Method
hf	-612.97	kJ/mol	Joback Method
hfus	39.24	kJ/mol	Joback Method
hvap	70.80	kJ/mol	Joback Method
log10ws	-7.07		Crippen Method
logp	6.665		Crippen Method
mcvol	306.560	ml/mol	McGowan Method
pc	1129.86	kPa	Joback Method
rinpol	2297.90		NIST Webbook
rinpol	2297.90		NIST Webbook
tb	787.94	K	Joback Method
tc	981.82	K	Joback Method
tf	481.54	K	Joback Method
vc	1.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1001.48	J/mol×K	787.94	Joback Method
cpg	1024.61	J/mol×K	820.25	Joback Method
cpg	1047.34	J/mol×K	852.57	Joback Method
cpg	1069.86	J/mol×K	884.88	Joback Method
cpg	1092.35	J/mol×K	917.20	Joback Method
cpg	1114.98	J/mol×K	949.51	Joback Method
cpg	1137.95	J/mol×K	981.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U414143&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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