

(R)-6-Methoxy-2,5,7,8-tetramethyl-2-((4R,8R)-4,8,1

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

CAS:

InChI=1S/C30H52O2/c1-21(2)13-10-14-22(3)15-11-16-23(4)17-12-19-30(8)20-18-27-26(

SCLDYIHKBCFVTE-ZRLASMASSA-N

C30H52O2

COc1c(C)c(C)c2c(c1C)CCC(C)(CCCC(C)CCCC(C)CCCC(C)C)O2

444.73

32466-45-8

Physical Properties

Property code	Value	Unit	Source
gf	110.70	kJ/mol	Joback Method
hf	-681.53	kJ/mol	Joback Method
hfus	53.89	kJ/mol	Joback Method
hvap	92.65	kJ/mol	Joback Method
log10ws	-10.34		Crippen Method
logp	9.143		Crippen Method
mcvol	410.680	ml/mol	McGowan Method
pc	753.08	kPa	Joback Method
rinpol	3056.30		NIST Webbook
rinpol	3052.00		NIST Webbook
rinpol	3056.30		NIST Webbook
rinpol	3052.00		NIST Webbook
tb	996.68	K	Joback Method
tc	1220.22	K	Joback Method
tf	559.00	K	Joback Method
vc	1.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1459.42	J/mol×K	996.68	Joback Method
cpg	1485.95	J/mol×K	1033.94	Joback Method
cpg	1511.96	J/mol×K	1071.19	Joback Method
cpg	1537.60	J/mol×K	1108.45	Joback Method
cpg	1563.05	J/mol×K	1145.70	Joback Method

cpg	1588.48	J/mol×K	1182.96	Joback Method
cpg	1614.06	J/mol×K	1220.22	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=C32466458&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
hvac:	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

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