

6-Methoxy-2,7,8-trimethyl-2-(4,8,12-trimethyltridecyl)tetrahydro-2H-pyran

Inchi: InChI=1S/C29H50O2/c1-21(2)12-9-13-22(3)14-10-15-23(4)16-11-18-29(7)19-17-26-20-28
InchiKey: YCYZEPRIDWTCRQ-UHFFFAOYSA-N
Formula: C29H50O2
SMILES: COc1cc2c(c(C)c1C)OC(C)(CCCC(C)CCCC(C)CCCC(C)C)CC2
Mol. weight [g/mol]: 430.71
CAS: 79306-82-4

Physical Properties

Property code	Value	Unit	Source
gf	111.91	kJ/mol	Joback Method
hf	-649.42	kJ/mol	Joback Method
hfus	51.69	kJ/mol	Joback Method
hvap	89.76	kJ/mol	Joback Method
log10ws	-9.86		Crippen Method
logp	8.835		Crippen Method
mcvol	396.590	ml/mol	McGowan Method
pc	801.15	kPa	Joback Method
rinpol	2984.30		NIST Webbook
tb	968.82	K	Joback Method
tc	1186.68	K	Joback Method
tf	535.21	K	Joback Method
vc	1.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1391.28	J/mol×K	968.82	Joback Method
cpg	1416.83	J/mol×K	1005.13	Joback Method
cpg	1441.82	J/mol×K	1041.44	Joback Method
cpg	1466.42	J/mol×K	1077.75	Joback Method
cpg	1490.77	J/mol×K	1114.06	Joback Method
cpg	1515.05	J/mol×K	1150.37	Joback Method
cpg	1539.41	J/mol×K	1186.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79306824&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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