(3S,8S,9S,10R,13R,14S,17R)-17-((2R,5R)-5,6-Dime

Inchi: InChI=1S/C29H50O/c1-19(2)20(3)8-9-21(4)25-12-13-26-24-11-10-22-18-23(30-7)14-16-2
InchiKey: AVIAVCZUGQDYFE-UHFFFAOYSA-N
Formula: C29H50O
SMILES: COC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)CCC(C)C(C)C)CCC32)C1
Mol. weight [g/mol]: 414.71
CAS: 29365-29-5

Physical Properties

Property code	Value	Unit	Source
gf	249.70	kJ/mol	Joback Method
hf	-513.78	kJ/mol	Joback Method
hfus	34.97	kJ/mol	Joback Method
hvap	79.63	kJ/mol	Joback Method
log10ws	-8.42		Crippen Method
logp	8.289		Crippen Method
mcvol	377.600	ml/mol	McGowan Method
pc	897.49	kPa	Joback Method
rinpol	3185.20		NIST Webbook
rinpol	3185.20		NIST Webbook
tb	922.94	K	Joback Method
tc	1146.34	K	Joback Method
tf	496.34	K	Joback Method
vc	1.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1397.36	J/mol×K	922.94	Joback Method
cpg	1429.41	J/mol×K	960.17	Joback Method
cpg	1461.48	J/mol×K	997.41	Joback Method
cpg	1493.88	J/mol×K	1034.64	Joback Method
cpg	1526.92	J/mol×K	1071.87	Joback Method
cpg	1560.93	J/mol×K	1109.10	Joback Method
cpg	1596.21	J/mol×K	1146.34	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29365295&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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