(E)-Taylopyran

Other names: 2,2,6-Trimethyl-3-[(E)(2-methylcyclopenta-2-en-1-ylidene)methyl]-3,4-dihydro-2H-pyran
Inchi: InChI=1S/C15H22O/c1-11-6-5-7-13(11)10-14-9-8-12(2)16-15(14,3)4/h6,8,10,14H,5,7,9H
InchiKey: MYZKUEUGZJCSJL-JWAFFJSPSA-N
Formula: C15H22O
SMILES: CC1=CCC(C=C2CCC=C2C)C(C)(C)O1
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	130.93	kJ/mol	Joback Method
hf	-186.24	kJ/mol	Joback Method
hfus	24.05	kJ/mol	Joback Method
hvap	55.72	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.372		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
rinpol	1536.00		NIST Webbook
rinpol	1536.00		NIST Webbook
tb	619.54	K	Joback Method
tc	850.80	K	Joback Method
tf	364.48	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.88	J/mol×K	619.54	Joback Method
cpg	537.53	J/mol×K	658.08	Joback Method
cpg	556.97	J/mol×K	696.63	Joback Method
cpg	575.34	J/mol×K	735.17	Joback Method
cpg	592.81	J/mol×K	773.72	Joback Method
cpg	609.55	J/mol×K	812.26	Joback Method
cpg	625.71	J/mol×K	850.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R407764&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume