Juneol

Inchi: InChI=1S/C15H26O/c1-10(2)13-9-8-12-7-5-6-11(3)15(12,4)14(13)16/h10,12-14,16H,3,5-9
InchiKey: WVGOZCUPNULHAM-GBJTYRQASA-N
Formula: C15H26O
SMILES: C=C1CCCC2CCC(C(C)C)C(O)C12C
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	41.43	kJ/mol	Joback Method
hf	-330.68	kJ/mol	Joback Method
hfus	17.73	kJ/mol	Joback Method
hvap	64.18	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.776		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinpol	1591.00		NIST Webbook
ripol	2087.00		NIST Webbook
tb	654.96	K	Joback Method
tc	859.10	K	Joback Method
tf	355.53	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.74	J/mol×K	654.96	Joback Method
cpg	616.91	J/mol×K	688.98	Joback Method
cpg	636.06	J/mol×K	723.01	Joback Method
cpg	654.29	J/mol×K	757.03	Joback Method
cpg	671.72	J/mol×K	791.05	Joback Method
cpg	688.46	J/mol×K	825.08	Joback Method
cpg	704.61	J/mol×K	859.10	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=R325870&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume