4-(3-Hydroxy-3-methylpent-4-enyl)-4a,8,8-trimethy (Laricsone)

Inchi: InChI=1S/C21H34O2/c1-7-20(5,23)12-8-10-16-15(2)14-17(22)18-19(3,4)11-9-13-21(16,1
InchiKey: VVFDQSZUGZLXAK-KPZFLHEBSA-N
Formula: C21H34O2
SMILES: C=CC(C)(O)CCCC1C(=C)CC(=O)C2C(C)(C)CCCC12C
Mol. weight [g/mol]: 318.49

Physical Properties

Property code	Value	Unit	Source
gf	56.99	kJ/mol	Joback Method
hf	-455.02	kJ/mol	Joback Method
hfus	21.31	kJ/mol	Joback Method
hvap	79.05	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	5.072		Crippen Method
mcvol	283.870	ml/mol	McGowan Method
pc	1431.55	kPa	Joback Method
rinpol	2189.00		NIST Webbook
rinpol	2189.00		NIST Webbook
tb	854.19	K	Joback Method
tc	1070.58	K	Joback Method
tf	530.93	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	962.65	J/mol×K	854.19	Joback Method
cpg	985.70	J/mol×K	890.26	Joback Method
cpg	1008.65	J/mol×K	926.32	Joback Method
cpg	1031.72	J/mol×K	962.39	Joback Method
cpg	1055.14	J/mol×K	998.45	Joback Method
cpg	1079.13	J/mol×K	1034.52	Joback Method
cpg	1103.94	J/mol×K	1070.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R635464&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