

«alpha»-Kessyl isovalerate

Inchi:	InChI=1S/C20H34O3/c1-12(2)9-18(21)22-17-11-20(6)15-8-7-13(3)14(15)10-16(17)19(4,5)
InchiKey:	AVQQNEGZVZHARMH-QELXSKCRSA-N
Formula:	C20H34O3
SMILES:	CC(C)CC(=O)OC1CC2(C)OC(C)(C)C1CC1C(C)CCC12
Mol. weight [g/mol]:	322.48

Physical Properties

Property code	Value	Unit	Source
gf	-100.83	kJ/mol	Joback Method
hf	-689.17	kJ/mol	Joback Method
hfus	34.59	kJ/mol	Joback Method
hvap	70.11	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	4.584		Crippen Method
mcvol	273.390	ml/mol	McGowan Method
pc	1402.74	kPa	Joback Method
rinsol	1986.00		NIST Webbook
tb	774.63	K	Joback Method
tc	991.54	K	Joback Method
tf	472.99	K	Joback Method
vc	1.034	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	915.26	J/mol×K	774.63	Joback Method
cpg	939.92	J/mol×K	810.78	Joback Method
cpg	963.97	J/mol×K	846.93	Joback Method
cpg	987.65	J/mol×K	883.09	Joback Method
cpg	1011.21	J/mol×K	919.24	Joback Method
cpg	1034.87	J/mol×K	955.39	Joback Method
cpg	1058.88	J/mol×K	991.54	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R224801&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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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