Methyl kolavenate

Inchi:	InChI=1S/C21H34O2/c1-15(14-19(22)23-6)10-12-20(4)17(3)11-13-21(5)16(2)8-7-9-18(20
InchiKey:	ULUVTDOVIRYSSF-CCEZHUSRSA-N
Formula:	C21H34O2
SMILES:	COC(=O)C=C(C)CCC1(C)C(C)CCC2(C)C(C)=CCCC21
Mol. weight [g/mol]:	318.49
CAS:	23527-24-4

Physical Properties

Property code	Value	Unit	Source
gf	30.72	kJ/mol	Joback Method
hf	-457.07	kJ/mol	Joback Method
hfus	30.07	kJ/mol	Joback Method
hvap	70.08	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	5.685		Crippen Method
mcvol	283.870	ml/mol	McGowan Method
pc	1345.70	kPa	Joback Method
rinpol	2359.00		NIST Webbook
rinpol	2372.20		NIST Webbook
rinpol	2372.20		NIST Webbook
tb	786.05	K	Joback Method
tc	1004.62	K	Joback Method
tf	453.95	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	901.63	J/mol×K	786.05	Joback Method
cpg	925.52	J/mol×K	822.48	Joback Method
cpg	948.94	J/mol×K	858.91	Joback Method
cpg	972.13	J/mol×K	895.34	Joback Method
cpg	995.33	J/mol×K	931.77	Joback Method
cpg	1018.77	J/mol×K	968.19	Joback Method

cpg	1042.70	J/mol×K	1004.62	Joback Method

Sources

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=C23527244&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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