Khusinol acetate

Inchi: InChI=1S/C17H26O2/c1-10(2)14-7-6-12(4)17-15(14)8-11(3)9-16(17)19-13(5)18/h8,10,14
InchiKey: FRBOFOXWQNXDHB-KZYLPZIUSA-N
Formula: C17H26O2
SMILES: C=C1CCC(C(C)C)C2C=C(C)CC(OC(C)=O)C12
Mol. weight [g/mol]: 262.39
CAS: 78405-34-2

Physical Properties

Property code	Value	Unit	Source
gf	-13.01	kJ/mol	Joback Method
hf	-433.46	kJ/mol	Joback Method
hfus	28.74	kJ/mol	Joback Method
hvap	63.21	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	4.123		Crippen Method
mcvol	227.510	ml/mol	McGowan Method
pc	1649.77	kPa	Joback Method
rinpol	1827.00		NIST Webbook
rinpol	1827.00		NIST Webbook
tb	688.73	K	Joback Method
tc	900.51	K	Joback Method
tf	378.79	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	673.05	J/mol×K	688.73	Joback Method
cpg	694.43	J/mol×K	724.03	Joback Method
cpg	714.48	J/mol×K	759.32	Joback Method
cpg	733.24	J/mol×K	794.62	Joback Method
cpg	750.74	J/mol×K	829.92	Joback Method
cpg	766.99	J/mol×K	865.21	Joback Method
cpg	782.02	J/mol×K	900.51	Joback Method

dvisc	0.0018083	Pa×s	378.79	Joback Method
dvisc	0.0011812	Pa×s	430.45	Joback Method
dvisc	0.0008453	Pa×s	482.10	Joback Method
dvisc	0.0006453	Pa×s	533.76	Joback Method
dvisc	0.0005168	Pa×s	585.42	Joback Method
dvisc	0.0004290	Pa×s	637.07	Joback Method
dvisc	0.0003662	Pa×s	688.73	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78405342&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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