

Euparin

Inchi:	InChI=1S/C14H16O2/c1-8(2)13-7-11-6-12(10(4)15)9(3)5-14(11)16-13/h5-6,13H,1,7H2,2-
InchiKey:	CJTGGNUUKMTUED-UHFFFAOYSA-N
Formula:	C14H16O2
SMILES:	<chem>C=C(C)C1Cc2cc(C(C)=O)c(C)cc2O1</chem>
Mol. weight [g/mol]:	216.28
CAS:	532-48-9

Physical Properties

Property code	Value	Unit	Source
gf	75.52	kJ/mol	Joback Method
hf	-186.31	kJ/mol	Joback Method
hfus	30.01	kJ/mol	Joback Method
hvap	61.60	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.077		Crippen Method
mcvol	176.640	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
rinpol	1858.80		NIST Webbook
rinpol	1858.80		NIST Webbook
tb	645.46	K	Joback Method
tc	869.95	K	Joback Method
tf	390.24	K	Joback Method
vc	0.677	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.55	J/mol×K	645.46	Joback Method
cpg	476.01	J/mol×K	682.88	Joback Method
cpg	490.47	J/mol×K	720.29	Joback Method
cpg	504.00	J/mol×K	757.71	Joback Method
cpg	516.66	J/mol×K	795.12	Joback Method
cpg	528.51	J/mol×K	832.54	Joback Method
cpg	539.63	J/mol×K	869.95	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=C532489&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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