

Hydrocinnamic acid, bornyl ester

Inchi:	InChI=1S/C19H26O2/c1-18(2)15-11-12-19(18,3)16(13-15)21-17(20)10-9-14-7-5-4-6-8-14
InchiKey:	FJRVVWLNKWCPLW-UHFFFAOYSA-N
Formula:	C19H26O2
SMILES:	CC1(C)C2CCC1(C)C(OC(=O)CCc1cccc1)C2
Mol. weight [g/mol]:	286.41
CAS:	326592-24-9

Physical Properties

Property code	Value	Unit	Source
gf	70.59	kJ/mol	Joback Method
hf	-314.52	kJ/mol	Joback Method
hfus	25.51	kJ/mol	Joback Method
hvap	66.40	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.377		Crippen Method
mcvol	240.530	ml/mol	McGowan Method
pc	1801.56	kPa	Joback Method
tb	745.98	K	Joback Method
tc	976.24	K	Joback Method
tf	474.15	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.12	J/molxK	745.98	Joback Method
cpg	758.55	J/molxK	784.36	Joback Method
cpg	779.44	J/molxK	822.73	Joback Method
cpg	800.12	J/molxK	861.11	Joback Method
cpg	820.87	J/molxK	899.49	Joback Method
cpg	842.00	J/molxK	937.86	Joback Method
cpg	863.81	J/molxK	976.24	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=C326592249&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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