

Amyloxy iso-eugenol

Inchi:	InChI=1S/C15H22O3/c1-4-6-7-9-18-14-11-13(16)15(17-3)10-12(14)8-5-2/h5,8,10-11,16H
InchiKey:	CKXKASLJCCTSEX-VMPITWQZSA-N
Formula:	C15H22O3
SMILES:	CC=Cc1cc(OC)c(O)cc1OCCCCC
Mol. weight [g/mol]:	250.33
CAS:	116632-98-5

Physical Properties

Property code	Value	Unit	Source
gf	-115.83	kJ/mol	Joback Method
hf	-463.87	kJ/mol	Joback Method
hfus	36.23	kJ/mol	Joback Method
hvap	70.38	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	4.003		Crippen Method
mcvol	211.760	ml/mol	McGowan Method
pc	2085.03	kPa	Joback Method
tb	708.86	K	Joback Method
tc	916.18	K	Joback Method
tf	461.37	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.03	J/molxK	708.86	Joback Method
cpg	604.41	J/molxK	743.41	Joback Method
cpg	618.99	J/molxK	777.97	Joback Method
cpg	632.84	J/molxK	812.52	Joback Method
cpg	646.00	J/molxK	847.08	Joback Method
cpg	658.54	J/molxK	881.63	Joback Method
cpg	670.49	J/molxK	916.18	Joback Method
dvisc	0.0002140	Paxs	461.37	Joback Method
dvisc	0.0000981	Paxs	502.62	Joback Method

dvisc	0.0000506	Paxs	543.87	Joback Method
dvisc	0.0000286	Paxs	585.12	Joback Method
dvisc	0.0000175	Paxs	626.36	Joback Method
dvisc	0.0000113	Paxs	667.61	Joback Method
dvisc	0.0000077	Paxs	708.86	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=C116632985&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	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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