

Cinnamic aldehyde, diethyl acetal

Inchi:	InChI=1S/C13H18O2/c1-3-14-13(15-4-2)11-10-12-8-6-5-7-9-12/h5-11,13H,3-4H2,1-2H3/
InchiKey:	VYKDEWVAUWARRX-ZHACJKMWSA-N
Formula:	C13H18O2
SMILES:	CCOC(C=Cc1ccccc1)OCC
Mol. weight [g/mol]:	206.28

Physical Properties

Property code	Value	Unit	Source
gf	38.77	kJ/mol	Joback Method
hf	-227.62	kJ/mol	Joback Method
hfus	22.52	kJ/mol	Joback Method
hvap	51.20	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	3.099		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2248.26	kPa	Joback Method
rinpol	1445.00		NIST Webbook
rinpol	1445.00		NIST Webbook
tb	572.08	K	Joback Method
tc	777.97	K	Joback Method
tf	287.07	K	Joback Method
vc	0.665	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.60	J/molxK	572.08	Joback Method
cpg	445.32	J/molxK	606.39	Joback Method
cpg	461.12	J/molxK	640.71	Joback Method
cpg	476.05	J/molxK	675.02	Joback Method
cpg	490.11	J/molxK	709.34	Joback Method
cpg	503.34	J/molxK	743.65	Joback Method
cpg	515.77	J/molxK	777.97	Joback Method
dvisc	0.0024436	Paxs	287.07	Joback Method

dvisc	0.0009903	Paxs	334.57	Joback Method
dvisc	0.0005024	Paxs	382.07	Joback Method
dvisc	0.0002962	Paxs	429.57	Joback Method
dvisc	0.0001940	Paxs	477.08	Joback Method
dvisc	0.0001371	Paxs	524.58	Joback Method
dvisc	0.0001027	Paxs	572.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R329461&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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