

Benzyl trans-4-coumarate

Inchi:	InChI=1S/C16H14O3/c17-15-9-6-13(7-10-15)8-11-16(18)19-12-14-4-2-1-3-5-14/h1-11,17
InchiKey:	RGZZCZQQPNJCPO-DHZHZOJOSA-N
Formula:	C16H14O3
SMILES:	O=C(C=Cc1ccc(O)cc1)OCc1ccccc1
Mol. weight [g/mol]:	254.28
CAS:	61844-62-0

Physical Properties

Property code	Value	Unit	Source
gf	0.34	kJ/mol	Joback Method
hf	-205.40	kJ/mol	Joback Method
hfus	34.05	kJ/mol	Joback Method
hvap	77.89	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.149		Crippen Method
mvol	197.790	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
rinpol	2490.20		NIST Webbook
rinpol	2490.20		NIST Webbook
tb	779.91	K	Joback Method
tc	1028.77	K	Joback Method
tf	501.72	K	Joback Method
vc	0.685	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.32	J/molxK	779.91	Joback Method
cpg	557.76	J/molxK	821.39	Joback Method
cpg	570.28	J/molxK	862.86	Joback Method
cpg	582.05	J/molxK	904.34	Joback Method
cpg	593.20	J/molxK	945.82	Joback Method
cpg	603.89	J/molxK	987.30	Joback Method
cpg	614.26	J/molxK	1028.77	Joback Method

dvisc	0.0001977	Paxs	501.72	Joback Method
dvisc	0.0000889	Paxs	548.09	Joback Method
dvisc	0.0000453	Paxs	594.45	Joback Method
dvisc	0.0000254	Paxs	640.82	Joback Method
dvisc	0.0000154	Paxs	687.18	Joback Method
dvisc	0.0000100	Paxs	733.54	Joback Method
dvisc	0.0000068	Paxs	779.91	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=C61844620&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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