

Benzyl (E)-ferulate

Inchi:	InChI=1S/C17H16O4/c1-20-16-11-13(7-9-15(16)18)8-10-17(19)21-12-14-5-3-2-4-6-14/h
InchiKey:	DZAPHTCUSDTZAT-CSKARUKUSA-N
Formula:	C17H16O4
SMILES:	COc1cc(C=CC(=O)OCc2ccccc2)ccc1O
Mol. weight [g/mol]:	284.31
CAS:	132335-97-8

Physical Properties

Property code	Value	Unit	Source
gf	-105.87	kJ/mol	Joback Method
hf	-369.73	kJ/mol	Joback Method
hfus	37.44	kJ/mol	Joback Method
hvap	83.19	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.157		Crippen Method
mvol	217.750	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
rinpol	2596.20		NIST Webbook
rinpol	2596.20		NIST Webbook
tb	830.19	K	Joback Method
tc	1071.69	K	Joback Method
tf	547.74	K	Joback Method
vc	0.759	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.82	J/molxK	830.19	Joback Method
cpg	636.24	J/molxK	870.44	Joback Method
cpg	648.81	J/molxK	910.69	Joback Method
cpg	660.61	J/molxK	950.94	Joback Method
cpg	671.77	J/molxK	991.19	Joback Method
cpg	682.39	J/molxK	1031.44	Joback Method
cpg	692.59	J/molxK	1071.69	Joback Method

dvisc	0.0000827	Paxs	547.74	Joback Method
dvisc	0.0000407	Paxs	594.82	Joback Method
dvisc	0.0000222	Paxs	641.89	Joback Method
dvisc	0.0000132	Paxs	688.96	Joback Method
dvisc	0.0000084	Paxs	736.04	Joback Method
dvisc	0.0000056	Paxs	783.12	Joback Method
dvisc	0.0000039	Paxs	830.19	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=C132335978&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
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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