

P-phenoxy-beta-methoxy phenetole

Inchi:	InChI=1S/C15H16O3/c1-16-11-12-17-13-7-9-15(10-8-13)18-14-5-3-2-4-6-14/h2-10H,11-
InchiKey:	ZUHYWLXZLTZZQF-UHFFFAOYSA-N
Formula:	C15H16O3
SMILES:	COCCOc1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]:	244.29
CAS:	57650-84-7

Physical Properties

Property code	Value	Unit	Source
gf	-24.39	kJ/mol	Joback Method
hf	-288.00	kJ/mol	Joback Method
hfus	25.86	kJ/mol	Joback Method
hvap	61.43	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	3.504		Crippen Method
mcvol	192.300	ml/mol	McGowan Method
pc	2351.92	kPa	Joback Method
tb	668.20	K	Joback Method
tc	894.06	K	Joback Method
tf	390.86	K	Joback Method
vc	0.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.78	J/molxK	668.20	Joback Method
cpg	572.25	J/molxK	856.42	Joback Method
cpg	560.15	J/molxK	818.78	Joback Method
cpg	546.96	J/molxK	781.13	Joback Method
cpg	532.68	J/molxK	743.49	Joback Method
cpg	517.29	J/molxK	705.84	Joback Method
cpg	583.28	J/molxK	894.06	Joback Method
dvisc	0.0000818	Paxs	668.20	Joback Method
dvisc	0.0001034	Paxs	621.98	Joback Method

dvisc	0.0001357	Paxs	575.75	Joback Method
dvisc	0.0001867	Paxs	529.53	Joback Method
dvisc	0.0002730	Paxs	483.31	Joback Method
dvisc	0.0004328	Paxs	437.08	Joback Method
dvisc	0.0007648	Paxs	390.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57650847&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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