

2-(Phenoxymethyl)benzoic acid

Other names:	Benzoic acid, 2-(phenoxymethyl)- o-(phenoxymethyl)benzoic acid
Inchi:	InChI=1S/C14H12O3/c15-14(16)13-9-5-4-6-11(13)10-17-12-7-2-1-3-8-12/h1-9H,10H2,(H
InchiKey:	YKNORODREYVARM-UHFFFAOYSA-N
Formula:	C14H12O3
SMILES:	O=C(O)c1ccccc1COc1ccccc1
Mol. weight [g/mol]:	228.24
CAS:	724-98-1

Physical Properties

Property code	Value	Unit	Source
gf	-88.55	kJ/mol	Joback Method
hf	-267.73	kJ/mol	Joback Method
hfus	26.58	kJ/mol	Joback Method
hvap	77.81	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	2.964		Crippen Method
mvol	173.910	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
tb	746.53	K	Joback Method
tc	970.42	K	Joback Method
tf	445.88	K	Joback Method
vc	0.646	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.37	J/molxK	746.53	Joback Method
cpg	514.90	J/molxK	933.11	Joback Method
cpg	506.70	J/molxK	895.79	Joback Method
cpg	497.68	J/molxK	858.48	Joback Method
cpg	487.82	J/molxK	821.16	Joback Method
cpg	477.06	J/molxK	783.85	Joback Method
cpg	522.33	J/molxK	970.42	Joback Method

dvisc	0.0000321	Paxs	746.53	Joback Method
dvisc	0.0000460	Paxs	696.42	Joback Method
dvisc	0.0000697	Paxs	646.31	Joback Method
dvisc	0.0001133	Paxs	596.20	Joback Method
dvisc	0.0002012	Paxs	546.10	Joback Method
dvisc	0.0004012	Paxs	495.99	Joback Method
dvisc	0.0009347	Paxs	445.88	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C724981&Units=SI

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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