Phenol, 4-(butoxymethyl)-2-methoxy-

Other names: 4-(butoxymethyl)-2-methoxyphenol
Vanillyl Butyl Ether
Inchi: InChI=1S/C12H18O3/c1-3-4-7-15-9-10-5-6-11(13)12(8-10)14-2/h5-6,8,13H,3-4,7,9H2,1-2
InchiKey: VLDFMKOUUQYFGF-UHFFFAOYSA-N
Formula: C12H18O3
SMILES: CCCCOCc1ccc(O)c(OC)c1
Mol. weight [g/mol]: 210.27
CAS: 82654-98-6

Physical Properties

Property code	Value	Unit	Source
gf	-211.68	kJ/mol	Joback Method
hf	-507.70	kJ/mol	Joback Method
hfus	28.65	kJ/mol	Joback Method
hvap	63.08	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.718		Crippen Method
mcvol	173.790	ml/mol	McGowan Method
pc	2659.77	kPa	Joback Method
rinpol	1651.00		NIST Webbook
tb	631.08	K	Joback Method
tc	838.65	K	Joback Method
tf	420.12	K	Joback Method
vc	0.602	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.98	J/mol×K	631.08	Joback Method
cpg	520.80	J/mol×K	804.06	Joback Method
cpg	509.20	J/mol×K	769.46	Joback Method
cpg	496.95	J/mol×K	734.87	Joback Method
cpg	484.03	J/mol×K	700.27	Joback Method
cpg	470.38	J/mol×K	665.68	Joback Method

cpg	531.80	J/mol×K	838.65	Joback Method
dvisc	0.0000181	Pa×s	631.08	Joback Method
dvisc	0.0000267	Pa×s	595.92	Joback Method
dvisc	0.0000415	Pa×s	560.76	Joback Method
dvisc	0.0000683	Pa×s	525.60	Joback Method
dvisc	0.0001208	Pa×s	490.44	Joback Method
dvisc	0.0002332	Pa×s	455.28	Joback Method
dvisc	0.0005028	Pa×s	420.12	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C82654986&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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