2-Dimethylamino-4-phenyl-2,6-xylenol

Inchi: InChI=1S/C16H19NO/c1-12-9-14(13-7-5-4-6-8-13)10-15(16(12)18)11-17(2)3/h4-10,18H,
InchiKey: ZUMGOSAJRWXKKE-UHFFFAOYSA-N
Formula: C16H19NO
SMILES: Cc1cc(-c2ccccc2)cc(CN(C)C)c1O
Mol. weight [g/mol]: 241.33
CAS: 116346-08-8

Physical Properties

Property code	Value	Unit	Source
gf	245.56	kJ/mol	Joback Method
hf	-33.23	kJ/mol	Joback Method
hfus	33.30	kJ/mol	Joback Method
hvap	72.14	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.429		Crippen Method
mcvol	204.630	ml/mol	McGowan Method
pc	2563.69	kPa	Joback Method
tb	721.86	K	Joback Method
tc	957.94	K	Joback Method
tf	492.15	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.70	J/mol×K	721.86	Joback Method
cpg	582.75	J/mol×K	761.21	Joback Method
cpg	597.75	J/mol×K	800.55	Joback Method
cpg	611.81	J/mol×K	839.90	Joback Method
cpg	625.07	J/mol×K	879.25	Joback Method
cpg	637.66	J/mol×K	918.59	Joback Method
cpg	649.70	J/mol×K	957.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116346088&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
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