2,4-BIS(DIMETHYLBENZYL)PHENOL

Other names: 2,4-Bis(dimethylbenzyl)phenol
2,4-Bis(1-methyl-1-phenylethyl)phenol
2,4-Bis(2-phenylpropan-2-yl)phenol
Inchi: InChI=1S/C24H26O/c1-23(2,18-11-7-5-8-12-18)20-15-16-22(25)21(17-20)24(3,4)19-13-9
InchiKey: FMUYQRFTLHAARI-UHFFFAOYSA-N
Formula: C24H26O
SMILES: CC(C)(c1ccccc1)c1ccc(O)c(C(C)(C)c2ccccc2)c1
Mol. weight [g/mol]: 330.47

Physical Properties

Property code	Value	Unit	Source
hf	2.78	kJ/mol	Cheméo Relay (1.0)
hfus	30.61	kJ/mol	Joback Method
hvap	128.49	kJ/mol	Cheméo Relay (1.0)
ie	7.73	eV	Cheméo Relay (1.0)
log10ws	-6.06		Cheméo Relay (1.0)
logp	6.044		Crippen Method
mcvol	283.610	ml/mol	McGowan Method
pc	1800.03	kPa	Joback Method
rinpol	2527.50		NIST Webbook
rinpol	2488.00		NIST Webbook
rinpol	2527.50		NIST Webbook
tb	641.80	K	Cheméo Relay (1.0)
tc	996.86	K	Cheméo Relay (1.0)
tf	405.04	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	887.30	J/mol×K	907.70	Joback Method
cpg	905.53	J/mol×K	952.26	Joback Method
cpg	923.03	J/mol×K	996.83	Joback Method
cpg	940.10	J/mol×K	1041.39	Joback Method
cpg	957.07	J/mol×K	1085.96	Joback Method

cpg	974.27	J/mol×K	1130.52	Joback Method
cpg	992.00	J/mol×K	1175.09	Joback Method
dvisc	0.0000631	Pa×s	568.58	Joback Method
dvisc	0.0000258	Pa×s	625.10	Joback Method
dvisc	0.0000123	Pa×s	681.62	Joback Method
dvisc	0.0000065	Pa×s	738.14	Joback Method
dvisc	0.0000038	Pa×s	794.66	Joback Method
dvisc	0.0000024	Pa×s	851.18	Joback Method
dvisc	0.0000016	Pa×s	907.70	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2772454&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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

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