5-Heptylresorcinol

Other names: 1,3-Benzenediol, 5-heptyl-
Inchi: InChI=1S/C13H20O2/c1-2-3-4-5-6-7-11-8-12(14)10-13(15)9-11/h8-10,14-15H,2-7H2,1H3
InchiKey: QENPJKGENOZEEJ-UHFFFAOYSA-N
Formula: C13H20O2
SMILES: CCCCCCCc1cc(O)cc(O)c1
Mol. weight [g/mol]: 208.30
CAS: 500-67-4

Physical Properties

Property code	Value	Unit	Source
gf	-138.25	kJ/mol	Joback Method
hf	-429.74	kJ/mol	Joback Method
hfus	35.03	kJ/mol	Joback Method
hvap	72.84	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.611		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2963.34	kPa	Joback Method
tb	684.76	K	Joback Method
tc	901.66	K	Joback Method
tf	486.13	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.57	J/mol×K	684.76	Joback Method
cpg	523.63	J/mol×K	720.91	Joback Method
cpg	536.95	J/mol×K	757.06	Joback Method
cpg	549.64	J/mol×K	793.21	Joback Method
cpg	561.82	J/mol×K	829.36	Joback Method
cpg	573.63	J/mol×K	865.51	Joback Method
cpg	585.19	J/mol×K	901.66	Joback Method
dvisc	0.0001000	Pa×s	486.13	Joback Method

dvisc	0.0000421	Pa×s	519.24	Joback Method
dvisc	0.0000197	Pa×s	552.34	Joback Method
dvisc	0.0000100	Pa×s	585.44	Joback Method
dvisc	0.0000055	Pa×s	618.55	Joback Method
dvisc	0.0000032	Pa×s	651.65	Joback Method
dvisc	0.0000020	Pa×s	684.76	Joback Method
hvapt	91.60	kJ/mol	473.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	490.00	K	1.90	NIST Webbook

Sources

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=C500674&Units=SI
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
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
hvapt: Enthalpy of vaporization at a given temperature
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

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume