5-Tridecylbenzene-1,3-diol

Inchi: InChI=1S/C19H32O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-17-14-18(20)16-19(21)15-17/h14-1
InchiKey: UXOGOSLLGMYCNL-UHFFFAOYSA-N
Formula: C19H32O2
SMILES: CCCCCCCCCCCCCc1cc(O)cc(O)c1
Mol. weight [g/mol]: 292.46
CAS: 5259-01-8

Physical Properties

Property code	Value	Unit	Source
gf	-87.73	kJ/mol	Joback Method
hf	-553.58	kJ/mol	Joback Method
hfus	50.57	kJ/mol	Joback Method
hvap	86.19	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	5.951		Crippen Method
mcvol	266.550	ml/mol	McGowan Method
pc	1717.45	kPa	Joback Method
rinpol	2591.00		NIST Webbook
rinpol	2591.00		NIST Webbook
tb	822.04	K	Joback Method
tc	1026.39	K	Joback Method
tf	553.75	K	Joback Method
vc	0.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	841.60	J/mol×K	822.04	Joback Method
cpg	922.41	J/mol×K	992.33	Joback Method
cpg	906.94	J/mol×K	958.27	Joback Method
cpg	891.24	J/mol×K	924.21	Joback Method
cpg	875.20	J/mol×K	890.16	Joback Method
cpg	858.69	J/mol×K	856.10	Joback Method
cpg	937.77	J/mol×K	1026.39	Joback Method

dvisc	0.0000003	Pa×s	822.04	Joback Method
dvisc	0.0000005	Pa×s	777.33	Joback Method
dvisc	0.0000010	Pa×s	732.61	Joback Method
dvisc	0.0000018	Pa×s	687.89	Joback Method
dvisc	0.0000037	Pa×s	643.18	Joback Method
dvisc	0.0000086	Pa×s	598.47	Joback Method
dvisc	0.0000225	Pa×s	553.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5259018&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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