4-(2,3,6-Trimethylphenyl)butan-2-ol

Inchi: InChI=1S/C13H20O/c1-9-5-6-10(2)13(12(9)4)8-7-11(3)14/h5-6,11,14H,7-8H2,1-4H3
InchiKey: IMXWSBUOJQZJJZ-UHFFFAOYSA-N
Formula: C13H20O
SMILES: Cc1ccc(C)c(CCC(C)O)c1C
Mol. weight [g/mol]: 192.30
CAS: 66248-70-2

Physical Properties

Property code	Value	Unit	Source
gf	2.84	kJ/mol	Joback Method
hf	-267.04	kJ/mol	Joback Method
hfus	22.86	kJ/mol	Joback Method
hvap	65.08	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	2.925		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
rinpol	1500.00		NIST Webbook
rinpol	1500.00		NIST Webbook
tb	630.20	K	Joback Method
tc	822.14	K	Joback Method
tf	346.07	K	Joback Method
vc	0.668	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.00	J/mol×K	630.20	Joback Method
cpg	520.26	J/mol×K	790.15	Joback Method
cpg	508.72	J/mol×K	758.16	Joback Method
cpg	496.55	J/mol×K	726.17	Joback Method
cpg	483.72	J/mol×K	694.18	Joback Method
cpg	470.21	J/mol×K	662.19	Joback Method
cpg	531.18	J/mol×K	822.14	Joback Method

dvisc	0.0000549	Pa×s	630.20	Joback Method
dvisc	0.0000826	Pa×s	582.85	Joback Method
dvisc	0.0001337	Pa×s	535.49	Joback Method
dvisc	0.0002374	Pa×s	488.14	Joback Method
dvisc	0.0004772	Pa×s	440.78	Joback Method
dvisc	0.0011346	Pa×s	393.43	Joback Method
dvisc	0.0034190	Pa×s	346.07	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66248702&Units=SI

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