1-(2,4-dimethylphenyl)ethanol

Inchi: InChI=1S/C10H14O/c1-7-4-5-10(9(3)11)8(2)6-7/h4-6,9,11H,1-3H3
InchiKey: DNHQUGRUHBFDFT-UHFFFAOYSA-N
Formula: C10H14O
SMILES: Cc1ccc(C(C)O)c(C)c1
Mol. weight [g/mol]: 150.22
CAS: 5379-19-1

Physical Properties

Property code	Value	Unit	Source
af	0.5937		Cheméo Relay (1.0)
gf	-12.79	kJ/mol	Joback Method
hf	-225.09	kJ/mol	Cheméo Relay (1.0)
hfus	15.48	kJ/mol	Joback Method
hvap	78.86	kJ/mol	Cheméo Relay (1.0)
ie	8.43	eV	Cheméo Relay (1.0)
log10ws	-1.66		Cheméo Relay (1.0)
logp	2.357		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
tb	497.46	K	Cheméo Relay (1.0)
tc	716.24	K	Cheméo Relay (1.0)
tf	333.79	K	Cheméo Relay (1.0)
vc	0.492	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.37	J/mol×K	556.58	Joback Method
cpg	323.63	J/mol×K	589.65	Joback Method
cpg	335.25	J/mol×K	622.73	Joback Method
cpg	346.27	J/mol×K	655.80	Joback Method
cpg	356.70	J/mol×K	688.88	Joback Method
cpg	366.57	J/mol×K	721.95	Joback Method
cpg	375.88	J/mol×K	755.02	Joback Method

dvisc	0.0084193	Pa×s	299.74	Joback Method
dvisc	0.0024711	Pa×s	342.55	Joback Method
dvisc	0.0009523	Pa×s	385.35	Joback Method
dvisc	0.0004441	Pa×s	428.16	Joback Method
dvisc	0.0002379	Pa×s	470.97	Joback Method
dvisc	0.0001414	Pa×s	513.77	Joback Method
dvisc	0.0000911	Pa×s	556.58	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5379191&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

af: Acentric Factor
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
ie: Ionization energy
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

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