1-Butyltetralin

Other names: Tetraline, 1-butyl
1-Butyl-1,2,3,4-tetrahydronaphthalene
Inchi: InChI=1S/C14H20/c1-2-3-7-12-9-6-10-13-8-4-5-11-14(12)13/h4-5,8,11-12H,2-3,6-7,9-10H
InchiKey: GCKPJUYBKVPDAU-UHFFFAOYSA-N
Formula: C14H20
SMILES: CCCCC1CCCc2ccccc21
Mol. weight [g/mol]: 188.31
CAS: 38857-76-0

Physical Properties

Property code	Value	Unit	Source
gf	218.43	kJ/mol	Joback Method
hf	-40.59	kJ/mol	Joback Method
hfus	21.70	kJ/mol	Joback Method
hvap	49.78	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	4.297		Crippen Method
mcvol	173.500	ml/mol	McGowan Method
pc	2287.14	kPa	Joback Method
rinpol	1489.19		NIST Webbook
rinpol	1533.35		NIST Webbook
rinpol	1496.00		NIST Webbook
tb	562.39	K	Joback Method
tc	779.06	K	Joback Method
tf	300.90	K	Joback Method
vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.06	J/mol×K	562.39	Joback Method
cpg	517.35	J/mol×K	742.95	Joback Method
cpg	502.09	J/mol×K	706.84	Joback Method
cpg	485.80	J/mol×K	670.73	Joback Method

cpg	468.40	J/mol×K	634.61	Joback Method
cpg	449.84	J/mol×K	598.50	Joback Method
cpg	531.63	J/mol×K	779.06	Joback Method
dvisc	0.0003095	Pa×s	562.39	Joback Method
dvisc	0.0003763	Pa×s	518.81	Joback Method
dvisc	0.0004743	Pa×s	475.23	Joback Method
dvisc	0.0006262	Pa×s	431.64	Joback Method
dvisc	0.0008802	Pa×s	388.06	Joback Method
dvisc	0.0013484	Pa×s	344.48	Joback Method
dvisc	0.0023374	Pa×s	300.90	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=C38857760&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

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