1-NAPHTHYL BUTYRATE

Other names:	«alpha»-Naphthyl butyrate
	n-Butyric acid «alpha»-naphthyl ester
	Butanoic acid, 1-naphthalenyl ester
	«alpha»-Naphthyl-n-butyrate
	Butyric acid, 1-naphthyl ester
Inchi:	InChI=1S/C14H14O2/c1-2-6-14(15)16-13-10-5-8-11-7-3-4-9-12(11)13/h3-5,7-10H,2,6H2,
InchiKey:	XIVJNRXPRQKFRZ-UHFFFAOYSA-N
Formula:	C14H14O2
SMILES:	CCCC(=O)Oc1cccc2ccccc12
Mol. weight [g/mol]:	214.26

Physical Properties

Property code	Value	Unit	Source
af	0.6216		Cheméo Relay (1.0)
hfus	25.47	kJ/mol	Joback Method
ie	7.83	eV	Cheméo Relay (1.0)
log10ws	-4.03		Cheméo Relay (1.0)
logp	3.545		Crippen Method
mcvol	172.340	ml/mol	McGowan Method
pc	2616.41	kPa	Joback Method
tb	579.96	K	Cheméo Relay (1.0)
tc	836.57	K	Cheméo Relay (1.0)
tf	289.24	K	Cheméo Relay (1.0)
vc	0.634	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.01	J/mol×K	646.65	Joback Method
cpg	448.60	J/mol×K	684.34	Joback Method
cpg	462.19	J/mol×K	722.03	Joback Method
cpg	474.83	J/mol×K	759.72	Joback Method
cpg	486.57	J/mol×K	797.41	Joback Method
cpg	497.48	J/mol×K	835.09	Joback Method

cpg	507.61	J/mol×K	872.78	Joback Method
dvisc	0.0014034	Pa×s	391.34	Joback Method
dvisc	0.0009208	Pa×s	433.89	Joback Method
dvisc	0.0006514	Pa×s	476.44	Joback Method
dvisc	0.0004877	Pa×s	519.00	Joback Method
dvisc	0.0003815	Pa×s	561.55	Joback Method
dvisc	0.0003090	Pa×s	604.10	Joback Method
dvisc	0.0002573	Pa×s	646.65	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	400.70	K	0.10	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3121708&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
hfus: Enthalpy of fusion 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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume