2-Naphthyl octanoate

Other names: Octanoic acid, 2-naphthalenyl ester
Octanoic acid, 2-naphthyl ester
Inchi: InChI=1S/C18H22O2/c1-2-3-4-5-6-11-18(19)20-17-13-12-15-9-7-8-10-16(15)14-17/h7-10
InchiKey: CXVZBUOSDMLXNK-UHFFFAOYSA-N
Formula: C18H22O2
SMILES: CCCCCCCC(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]: 270.37
CAS: 10251-17-9

Physical Properties

Property code	Value	Unit	Source
gf	76.19	kJ/mol	Joback Method
hf	-243.52	kJ/mol	Joback Method
hfus	35.83	kJ/mol	Joback Method
hvap	69.40	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	5.106		Crippen Method
mcvol	228.700	ml/mol	McGowan Method
pc	1827.85	kPa	Joback Method
rinpol	2211.00		NIST Webbook
rinpol	2211.00		NIST Webbook
tb	738.17	K	Joback Method
tc	950.21	K	Joback Method
tf	436.42	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.16	J/mol×K	738.17	Joback Method
cpg	661.36	J/mol×K	773.51	Joback Method
cpg	676.53	J/mol×K	808.85	Joback Method
cpg	690.72	J/mol×K	844.19	Joback Method
cpg	703.99	J/mol×K	879.53	Joback Method

cpg	716.40	J/mol×K	914.87	Joback Method
cpg	728.02	J/mol×K	950.21	Joback Method
dvisc	0.0012149	Pa×s	436.42	Joback Method
dvisc	0.0007463	Pa×s	486.71	Joback Method
dvisc	0.0005022	Pa×s	537.00	Joback Method
dvisc	0.0003617	Pa×s	587.29	Joback Method
dvisc	0.0002744	Pa×s	637.59	Joback Method
dvisc	0.0002167	Pa×s	687.88	Joback Method
dvisc	0.0001767	Pa×s	738.17	Joback Method

Sources

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=C10251179&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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