

Valeric acid, 2-naphthyl ester

Inchi:	InChI=1S/C15H16O2/c1-2-3-8-15(16)17-14-10-9-12-6-4-5-7-13(12)11-14/h4-7,9-11H,2-3
InchiKey:	ZMPGOHSLJBONFZ-UHFFFAOYSA-N
Formula:	C15H16O2
SMILES:	CCCCC(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]:	228.29

Physical Properties

Property code	Value	Unit	Source
gf	50.93	kJ/mol	Joback Method
hf	-181.60	kJ/mol	Joback Method
hfus	28.06	kJ/mol	Joback Method
hvap	62.72	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	3.935		Crippen Method
mcvol	186.430	ml/mol	McGowan Method
pc	2377.22	kPa	Joback Method
rinsol	1893.00		NIST Webbook
tb	669.53	K	Joback Method
tc	891.56	K	Joback Method
tf	402.61	K	Joback Method
vc	0.714	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.87	J/molxK	669.53	Joback Method
cpg	499.97	J/molxK	706.54	Joback Method
cpg	514.06	J/molxK	743.54	Joback Method
cpg	527.18	J/molxK	780.55	Joback Method
cpg	539.41	J/molxK	817.55	Joback Method
cpg	550.78	J/molxK	854.56	Joback Method
cpg	561.37	J/molxK	891.56	Joback Method
dvisc	0.0013729	Paxs	402.61	Joback Method
dvisc	0.0008852	Paxs	447.10	Joback Method

dvisc	0.0006179	Paxs	491.58	Joback Method
dvisc	0.0004579	Paxs	536.07	Joback Method
dvisc	0.0003552	Paxs	580.56	Joback Method
dvisc	0.0002857	Paxs	625.04	Joback Method
dvisc	0.0002366	Paxs	669.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307990&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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