

2-Methylpropionic acid, 2-naphthyl ester

Inchi:	InChI=1S/C14H14O2/c1-10(2)14(15)16-13-8-7-11-5-3-4-6-12(11)9-13/h3-10H,1-2H3
InchiKey:	RVFNBABJYWYXFR-UHFFFAOYSA-N
Formula:	C14H14O2
SMILES:	CC(C)C(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]:	214.26

Physical Properties

Property code	Value	Unit	Source
gf	40.07	kJ/mol	Joback Method
hf	-166.24	kJ/mol	Joback Method
hfus	21.95	kJ/mol	Joback Method
hvap	60.10	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.401		Crippen Method
mcvol	172.340	ml/mol	McGowan Method
pc	2637.96	kPa	Joback Method
rinpol	1724.00		NIST Webbook
tb	646.21	K	Joback Method
tc	877.01	K	Joback Method
tf	376.34	K	Joback Method
vc	0.651	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.50	J/molxK	646.21	Joback Method
cpg	449.44	J/molxK	684.68	Joback Method
cpg	463.31	J/molxK	723.14	Joback Method
cpg	476.19	J/molxK	761.61	Joback Method
cpg	488.12	J/molxK	800.08	Joback Method
cpg	499.18	J/molxK	838.55	Joback Method
cpg	509.41	J/molxK	877.01	Joback Method
dvisc	0.0016107	Paxs	376.34	Joback Method
dvisc	0.0009890	Paxs	421.32	Joback Method

dvisc	0.0006672	Paxs	466.30	Joback Method
dvisc	0.0004823	Paxs	511.28	Joback Method
dvisc	0.0003675	Paxs	556.25	Joback Method
dvisc	0.0002916	Paxs	601.23	Joback Method
dvisc	0.0002390	Paxs	646.21	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=U308021&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
mccvol:	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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