

4-Chlorobutyric acid, 2-naphthyl ester

Inchi:	InChI=1S/C14H13ClO2/c15-9-3-6-14(16)17-13-8-7-11-4-1-2-5-12(11)10-13/h1-2,4-5,7-8,
InchiKey:	KNSGPNGISXLZHO-UHFFFAOYSA-N
Formula:	C14H13ClO2
SMILES:	O=C(CCCCl)Oc1ccc2ccccc2c1
Mol. weight [g/mol]:	248.71

Physical Properties

Property code	Value	Unit	Source
gf	30.58	kJ/mol	Joback Method
hf	-176.70	kJ/mol	Joback Method
hfus	29.67	kJ/mol	Joback Method
hvap	64.88	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.764		Crippen Method
mvol	184.580	ml/mol	McGowan Method
pc	2520.12	kPa	Joback Method
rinpol	2045.00		NIST Webbook
rinpol	2045.00		NIST Webbook
tb	684.08	K	Joback Method
tc	913.20	K	Joback Method
tf	421.26	K	Joback Method
vc	0.707	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.37	J/mol×K	684.08	Joback Method
cpg	472.81	J/mol×K	722.27	Joback Method
cpg	485.27	J/mol×K	760.45	Joback Method
cpg	496.82	J/mol×K	798.64	Joback Method
cpg	507.52	J/mol×K	836.83	Joback Method
cpg	517.42	J/mol×K	875.01	Joback Method
cpg	526.59	J/mol×K	913.20	Joback Method
dvisc	0.0013437	Paxs	421.26	Joback Method

dvisc	0.0008880	Paxs	465.06	Joback Method
dvisc	0.0006302	Paxs	508.87	Joback Method
dvisc	0.0004722	Paxs	552.67	Joback Method
dvisc	0.0003691	Paxs	596.47	Joback Method
dvisc	0.0002985	Paxs	640.28	Joback Method
dvisc	0.0002480	Paxs	684.08	Joback Method

Sources

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=U307605&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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