

2-Bromopropionic acid, 2-naphthyl ester

Inchi:	InChI=1S/C13H11BrO2/c1-9(14)13(15)16-12-7-6-10-4-2-3-5-11(10)8-12/h2-9H,1H3
InchiKey:	RBWIIQIGQLKDLAM-UHFFFAOYSA-N
Formula:	C13H11BrO2
SMILES:	CC(Br)C(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]:	279.13

Physical Properties

Property code	Value	Unit	Source
gf	45.97	kJ/mol	Joback Method
hf	-119.27	kJ/mol	Joback Method
hfus	24.65	kJ/mol	Joback Method
hvap	64.31	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	3.529		Crippen Method
mcvol	175.750	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
rinsol	1913.00		NIST Webbook
tb	689.49	K	Joback Method
tc	936.33	K	Joback Method
tf	424.87	K	Joback Method
vc	0.657	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.35	J/molxK	689.49	Joback Method
cpg	474.52	J/molxK	895.19	Joback Method
cpg	465.40	J/molxK	854.05	Joback Method
cpg	455.51	J/molxK	812.91	Joback Method
cpg	444.76	J/molxK	771.77	Joback Method
cpg	433.06	J/molxK	730.63	Joback Method
cpg	482.94	J/molxK	936.33	Joback Method
dvisc	0.0002525	Paxs	689.49	Joback Method
dvisc	0.0003051	Paxs	645.39	Joback Method

dvisc	0.0003791	Paxs	601.28	Joback Method
dvisc	0.0004874	Paxs	557.18	Joback Method
dvisc	0.0006545	Paxs	513.08	Joback Method
dvisc	0.0009288	Paxs	468.97	Joback Method
dvisc	0.0014176	Paxs	424.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308028&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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