4-Bromobutyric acid, 2-naphthyl ester

Inchi: InChI=1S/C14H13BrO2/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: WROMMFRWIWBKCJ-UHFFFAOYSA-N
Formula: C14H13BrO2
SMILES: O=C(CCCBr)Oc1ccc2ccccc2c1
Mol. weight [g/mol]: 293.16

Physical Properties

Property code	Value	Unit	Source
gf	56.83	kJ/mol	Joback Method
hf	-134.63	kJ/mol	Joback Method
hfus	30.76	kJ/mol	Joback Method
hvap	66.93	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	3.920		Crippen Method
mcvol	189.840	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
rinpol	2156.00		NIST Webbook
rinpol	2156.00		NIST Webbook
tb	712.81	K	Joback Method
tc	949.71	K	Joback Method
tf	451.14	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.43	J/mol×K	712.81	Joback Method
cpg	483.43	J/mol×K	752.29	Joback Method
cpg	495.46	J/mol×K	791.78	Joback Method
cpg	506.59	J/mol×K	831.26	Joback Method
cpg	516.90	J/mol×K	870.75	Joback Method
cpg	526.46	J/mol×K	910.23	Joback Method
cpg	535.36	J/mol×K	949.71	Joback Method
dvisc	0.0012166	Pa×s	451.14	Joback Method

dvisc	0.0008285	Pa×s	494.75	Joback Method
dvisc	0.0006004	Pa×s	538.36	Joback Method
dvisc	0.0004567	Pa×s	581.98	Joback Method
dvisc	0.0003608	Pa×s	625.59	Joback Method
dvisc	0.0002940	Pa×s	669.20	Joback Method
dvisc	0.0002456	Pa×s	712.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307613&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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