6-Bromohexanoic acid, 2-naphthyl ester

Inchi: InChI=1S/C16H17BrO2/c17-11-5-1-2-8-16(18)19-15-10-9-13-6-3-4-7-14(13)12-15/h3-4,6
InchiKey: XQCOAGSPTVBHIO-UHFFFAOYSA-N
Formula: C16H17BrO2
SMILES: O=C(CCCCCBr)Oc1ccc2ccccc2c1
Mol. weight [g/mol]: 321.21

Physical Properties

Property code	Value	Unit	Source
gf	73.67	kJ/mol	Joback Method
hf	-175.91	kJ/mol	Joback Method
hfus	35.94	kJ/mol	Joback Method
hvap	71.38	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	4.700		Crippen Method
mcvol	218.020	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
rinpol	2418.00		NIST Webbook
rinpol	2418.00		NIST Webbook
tb	758.57	K	Joback Method
tc	986.97	K	Joback Method
tf	473.68	K	Joback Method
vc	0.832	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.50	J/mol×K	758.57	Joback Method
cpg	589.40	J/mol×K	796.64	Joback Method
cpg	602.33	J/mol×K	834.70	Joback Method
cpg	614.36	J/mol×K	872.77	Joback Method
cpg	625.57	J/mol×K	910.84	Joback Method
cpg	636.03	J/mol×K	948.91	Joback Method
cpg	645.82	J/mol×K	986.97	Joback Method
dvisc	0.0010829	Pa×s	473.68	Joback Method

dvisc	0.0007155	Pa×s	521.16	Joback Method
dvisc	0.0005066	Pa×s	568.64	Joback Method
dvisc	0.0003783	Pa×s	616.12	Joback Method
dvisc	0.0002946	Pa×s	663.61	Joback Method
dvisc	0.0002372	Pa×s	711.09	Joback Method
dvisc	0.0001962	Pa×s	758.57	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=U307620&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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