2-Bromobenzoic acid, undec-2-enyl ester

Inchi: InChI=1S/C18H25BrO2/c1-2-3-4-5-6-7-8-9-12-15-21-18(20)16-13-10-11-14-17(16)19/h9-
InchiKey: JENAWSKCVBMMMU-FMIVXFBMSA-N
Formula: C18H25BrO2
SMILES: CCCCCCCCC=CCOC(=O)c1ccccc1Br
Mol. weight [g/mol]: 353.29

Physical Properties

Property code	Value	Unit	Source
gf	64.08	kJ/mol	Joback Method
hf	-291.04	kJ/mol	Joback Method
hfus	44.30	kJ/mol	Joback Method
hvap	74.15	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	5.913		Crippen Method
mcvol	261.360	ml/mol	McGowan Method
pc	1648.43	kPa	Joback Method
rinpol	2327.00		NIST Webbook
rinpol	2327.00		NIST Webbook
tb	789.51	K	Joback Method
tc	998.63	K	Joback Method
tf	458.44	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.35	J/mol×K	789.51	Joback Method
cpg	800.58	J/mol×K	963.78	Joback Method
cpg	788.44	J/mol×K	928.92	Joback Method
cpg	775.51	J/mol×K	894.07	Joback Method
cpg	761.72	J/mol×K	859.22	Joback Method
cpg	747.02	J/mol×K	824.36	Joback Method
cpg	811.97	J/mol×K	998.63	Joback Method
dvisc	0.0000696	Pa×s	789.51	Joback Method

dvisc	0.0000892	Pa×s	734.33	Joback Method
dvisc	0.0001192	Pa×s	679.15	Joback Method
dvisc	0.0001676	Pa×s	623.97	Joback Method
dvisc	0.0002517	Pa×s	568.80	Joback Method
dvisc	0.0004127	Pa×s	513.62	Joback Method
dvisc	0.0007619	Pa×s	458.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299399&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

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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