

4-Bromobenzoic acid, undec-2-enyl ester

Inchi:	InChI=1S/C18H25BrO2/c1-2-3-4-5-6-7-8-9-10-15-21-18(20)16-11-13-17(19)14-12-16/h9-
InchiKey:	PTJQZPBXJDRGFY-MDZDMXLPSA-N
Formula:	C18H25BrO2
SMILES:	CCCCCCCCC=CCOC(=O)c1ccc(Br)cc1
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
mvol	261.360	ml/mol	McGowan Method
pc	1648.43	kPa	Joback Method
rinpol	2325.00		NIST Webbook
rinpol	2325.00		NIST Webbook
tb	789.51	K	Joback Method
tc	998.63	K	Joback Method
tf	458.44	K	Joback Method
vc	1.002	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.35	J/molxK	789.51	Joback Method
cpg	747.02	J/molxK	824.36	Joback Method
cpg	761.72	J/molxK	859.22	Joback Method
cpg	775.51	J/molxK	894.07	Joback Method
cpg	788.44	J/molxK	928.92	Joback Method
cpg	800.58	J/molxK	963.78	Joback Method
cpg	811.97	J/molxK	998.63	Joback Method
dvisc	0.0007619	Paxs	458.44	Joback Method

dvisc	0.0004127	Paxs	513.62	Joback Method
dvisc	0.0002517	Paxs	568.80	Joback Method
dvisc	0.0001676	Paxs	623.97	Joback Method
dvisc	0.0001192	Paxs	679.15	Joback Method
dvisc	0.0000892	Paxs	734.33	Joback Method
dvisc	0.0000696	Paxs	789.51	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
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=U299251&Units=SI

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
log_p:	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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