

n-Butyl 2-(4-bromophenyl)acetate

Inchi:	InChI=1S/C12H15BrO2/c1-2-3-8-15-12(14)9-10-4-6-11(13)7-5-10/h4-7H,2-3,8-9H2,1H3
InchiKey:	MMLFPGZTRUZTEV-UHFFFAOYSA-N
Formula:	C12H15BrO2
SMILES:	CCCCOC(=O)Cc1ccc(Br)cc1
Mol. weight [g/mol]:	271.15

Physical Properties

Property code	Value	Unit	Source
gf	-66.66	kJ/mol	Joback Method
hf	-284.42	kJ/mol	Joback Method
hfus	28.56	kJ/mol	Joback Method
hvap	60.84	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.335		Crippen Method
mcvol	181.120	ml/mol	McGowan Method
pc	2659.77	kPa	Joback Method
rinpol	1781.00		NIST Webbook
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tb	648.07	K	Joback Method
tc	867.01	K	Joback Method
tf	395.90	K	Joback Method
vc	0.685	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.91	J/molxK	648.07	Joback Method
cpg	447.63	J/molxK	684.56	Joback Method
cpg	460.50	J/molxK	721.05	Joback Method
cpg	472.52	J/molxK	757.54	Joback Method
cpg	483.75	J/molxK	794.03	Joback Method
cpg	494.20	J/molxK	830.52	Joback Method
cpg	503.90	J/molxK	867.01	Joback Method
dvisc	0.0013207	Paxs	395.90	Joback Method

dvisc	0.0007985	Paxs	437.93	Joback Method
dvisc	0.0005273	Paxs	479.96	Joback Method
dvisc	0.0003722	Paxs	521.99	Joback Method
dvisc	0.0002768	Paxs	564.01	Joback Method
dvisc	0.0002144	Paxs	606.04	Joback Method
dvisc	0.0001717	Paxs	648.07	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U372918&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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