

Heptyl 2-bromobutanoate

Inchi:	InChI=1S/C11H21BrO2/c1-3-5-6-7-8-9-14-11(13)10(12)4-2/h10H,3-9H2,1-2H3
InchiKey:	MTMOXPALHHFPIA-UHFFFAOYSA-N
Formula:	C11H21BrO2
SMILES:	CCCCCCCOC(=O)C(Br)CC
Mol. weight [g/mol]:	265.19

Physical Properties

Property code	Value	Unit	Source
gf	-180.30	kJ/mol	Joback Method
hf	-494.12	kJ/mol	Joback Method
hfus	28.80	kJ/mol	Joback Method
hvap	55.28	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.674		Crippen Method
mcvol	190.790	ml/mol	McGowan Method
pc	2161.32	kPa	Joback Method
rinpol	1503.00		NIST Webbook
rinpol	1503.00		NIST Webbook
tb	593.09	K	Joback Method
tc	779.97	K	Joback Method
tf	330.69	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.31	J/molxK	593.09	Joback Method
cpg	476.91	J/molxK	624.24	Joback Method
cpg	490.82	J/molxK	655.38	Joback Method
cpg	504.08	J/molxK	686.53	Joback Method
cpg	516.68	J/molxK	717.68	Joback Method
cpg	528.64	J/molxK	748.82	Joback Method
cpg	539.99	J/molxK	779.97	Joback Method
dvisc	0.0027963	Paxs	330.69	Joback Method

dvisc	0.0013618	Paxs	374.42	Joback Method
dvisc	0.0007709	Paxs	418.16	Joback Method
dvisc	0.0004860	Paxs	461.89	Joback Method
dvisc	0.0003319	Paxs	505.62	Joback Method
dvisc	0.0002408	Paxs	549.36	Joback Method
dvisc	0.0001832	Paxs	593.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R23362&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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