Decyl 2-bromobutanoate

Inchi: InChI=1S/C14H27BrO2/c1-3-5-6-7-8-9-10-11-12-17-14(16)13(15)4-2/h13H,3-12H2,1-2H
InchiKey: PXWPPMIZSAEDJP-UHFFFAOYSA-N
Formula: C14H27BrO2
SMILES: CCCCCCCCCCOC(=O)C(Br)CC
Mol. weight [g/mol]: 307.27

Physical Properties

Property code	Value	Unit	Source
gf	-155.04	kJ/mol	Joback Method
hf	-556.04	kJ/mol	Joback Method
hfus	36.57	kJ/mol	Joback Method
hvap	61.96	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.844		Crippen Method
mcvol	233.060	ml/mol	McGowan Method
pc	1681.03	kPa	Joback Method
rinpol	1800.00		NIST Webbook
rinpol	1800.00		NIST Webbook
tb	661.73	K	Joback Method
tc	843.92	K	Joback Method
tf	364.50	K	Joback Method
vc	0.899	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.33	J/mol×K	661.73	Joback Method
cpg	691.90	J/mol×K	813.55	Joback Method
cpg	678.66	J/mol×K	783.19	Joback Method
cpg	664.70	J/mol×K	752.82	Joback Method
cpg	650.01	J/mol×K	722.46	Joback Method
cpg	634.56	J/mol×K	692.09	Joback Method
cpg	704.44	J/mol×K	843.92	Joback Method
dvisc	0.0001254	Pa×s	661.73	Joback Method

dvisc	0.0001665	Pa×s	612.19	Joback Method
dvisc	0.0002325	Pa×s	562.65	Joback Method
dvisc	0.0003461	Pa×s	513.12	Joback Method
dvisc	0.0005611	Pa×s	463.58	Joback Method
dvisc	0.0010210	Pa×s	414.04	Joback Method
dvisc	0.0021862	Pa×s	364.50	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=R23287&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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