Dodecyl 2-bromobutanoate

Inchi: InChI=1S/C16H31BrO2/c1-3-5-6-7-8-9-10-11-12-13-14-19-16(18)15(17)4-2/h15H,3-14H2
InchiKey: NXCHIIAWZIHPAX-UHFFFAOYSA-N
Formula: C16H31BrO2
SMILES: CCCCCCCCCCCCOC(=O)C(Br)CC
Mol. weight [g/mol]: 335.32

Physical Properties

Property code	Value	Unit	Source
gf	-138.20	kJ/mol	Joback Method
hf	-597.32	kJ/mol	Joback Method
hfus	41.74	kJ/mol	Joback Method
hvap	66.41	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	5.624		Crippen Method
mcvol	261.240	ml/mol	McGowan Method
pc	1444.64	kPa	Joback Method
rinpol	1999.00		NIST Webbook
rinpol	1999.00		NIST Webbook
tb	707.49	K	Joback Method
tc	888.41	K	Joback Method
tf	387.04	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	729.06	J/mol×K	707.49	Joback Method
cpg	746.14	J/mol×K	737.64	Joback Method
cpg	762.37	J/mol×K	767.80	Joback Method
cpg	777.79	J/mol×K	797.95	Joback Method
cpg	792.42	J/mol×K	828.10	Joback Method
cpg	806.28	J/mol×K	858.25	Joback Method
cpg	819.40	J/mol×K	888.41	Joback Method
dvisc	0.0017995	Pa×s	387.04	Joback Method

dvisc	0.0008202	Pa×s	440.45	Joback Method
dvisc	0.0004431	Pa×s	493.86	Joback Method
dvisc	0.0002699	Pa×s	547.26	Joback Method
dvisc	0.0001796	Pa×s	600.67	Joback Method
dvisc	0.0001277	Pa×s	654.08	Joback Method
dvisc	0.0000956	Pa×s	707.49	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R23326&Units=SI

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