Dodecyl 2-bromopropanoate

Inchi: InChI=1S/C15H29BrO2/c1-3-4-5-6-7-8-9-10-11-12-13-18-15(17)14(2)16/h14H,3-13H2,1-
InchiKey: RXTSHIDRCASANN-UHFFFAOYSA-N
Formula: C15H29BrO2
SMILES: CCCCCCCCCCCCOC(=O)C(C)Br
Mol. weight [g/mol]: 321.29

Physical Properties

Property code	Value	Unit	Source
gf	-146.62	kJ/mol	Joback Method
hf	-576.68	kJ/mol	Joback Method
hfus	39.15	kJ/mol	Joback Method
hvap	64.19	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	5.234		Crippen Method
mcvol	247.150	ml/mol	McGowan Method
pc	1556.12	kPa	Joback Method
rinpol	1911.00		NIST Webbook
rinpol	1911.00		NIST Webbook
tb	684.61	K	Joback Method
tc	865.94	K	Joback Method
tf	375.77	K	Joback Method
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	673.08	J/mol×K	684.61	Joback Method
cpg	748.56	J/mol×K	835.72	Joback Method
cpg	734.99	J/mol×K	805.50	Joback Method
cpg	720.68	J/mol×K	775.28	Joback Method
cpg	705.61	J/mol×K	745.05	Joback Method
cpg	689.75	J/mol×K	714.83	Joback Method
cpg	761.41	J/mol×K	865.94	Joback Method
dvisc	0.0001097	Pa×s	684.61	Joback Method

dvisc	0.0001461	Pa×s	633.14	Joback Method
dvisc	0.0002047	Pa×s	581.66	Joback Method
dvisc	0.0003063	Pa×s	530.19	Joback Method
dvisc	0.0004997	Pa×s	478.72	Joback Method
dvisc	0.0009173	Pa×s	427.24	Joback Method
dvisc	0.0019888	Pa×s	375.77	Joback Method

Sources

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=R23330&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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