2- Bromopropionic acid, octyl ester

Other names: Octyl 2-bromopropanoate
Inchi: InChI=1S/C11H21BrO2/c1-3-4-5-6-7-8-9-14-11(13)10(2)12/h10H,3-9H2,1-2H3
InchiKey: BOCFEZOZUMAGFA-UHFFFAOYSA-N
Formula: C11H21BrO2
SMILES: CCCCCCCCOC(=O)C(C)Br
Mol. weight [g/mol]: 265.19
CAS: 24625-82-9

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	1419.70		NIST Webbook
rinpol	1511.00		NIST Webbook
rinpol	1419.70		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/mol×K	593.09	Joback Method
cpg	476.91	J/mol×K	624.24	Joback Method
cpg	490.82	J/mol×K	655.38	Joback Method
cpg	504.08	J/mol×K	686.53	Joback Method
cpg	516.68	J/mol×K	717.68	Joback Method

cpg	528.64	J/mol×K	748.82	Joback Method
cpg	539.99	J/mol×K	779.97	Joback Method
dvisc	0.0027963	Pa×s	330.69	Joback Method
dvisc	0.0013618	Pa×s	374.42	Joback Method
dvisc	0.0007709	Pa×s	418.16	Joback Method
dvisc	0.0004860	Pa×s	461.89	Joback Method
dvisc	0.0003319	Pa×s	505.62	Joback Method
dvisc	0.0002408	Pa×s	549.36	Joback Method
dvisc	0.0001832	Pa×s	593.09	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C24625829&Units=SI
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

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