Propanoic acid, 3-bromo, isohexyl ester

Other names: Propanoic acid, 3-bromo, 4-methylpentyl ester
Inchi: InChI=1S/C9H17BrO2/c1-8(2)4-3-7-12-9(11)5-6-10/h8H,3-7H2,1-2H3
InchiKey: WGZWVZAMWFMCEG-UHFFFAOYSA-N
Formula: C9H17BrO2
SMILES: CC(C)CCCOC(=O)CCBr
Mol. weight [g/mol]: 237.13

Physical Properties

Property code	Value	Unit	Source
gf	-197.14	kJ/mol	Joback Method
hf	-452.84	kJ/mol	Joback Method
hfus	23.62	kJ/mol	Joback Method
hvap	50.83	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.751		Crippen Method
mcvol	162.610	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
rinpol	1330.00		NIST Webbook
rinpol	1330.00		NIST Webbook
ripol	1776.00		NIST Webbook
tb	547.33	K	Joback Method
tc	738.62	K	Joback Method
tf	308.15	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.10	J/mol×K	547.33	Joback Method
cpg	379.22	J/mol×K	579.21	Joback Method
cpg	391.74	J/mol×K	611.09	Joback Method
cpg	403.67	J/mol×K	642.98	Joback Method
cpg	415.02	J/mol×K	674.86	Joback Method
cpg	425.81	J/mol×K	706.74	Joback Method

cpg	436.04	J/mol×K	738.62	Joback Method
dvisc	0.0031707	Pa×s	308.15	Joback Method
dvisc	0.0015948	Pa×s	348.01	Joback Method
dvisc	0.0009238	Pa×s	387.88	Joback Method
dvisc	0.0005925	Pa×s	427.74	Joback Method
dvisc	0.0004099	Pa×s	467.60	Joback Method
dvisc	0.0003004	Pa×s	507.47	Joback Method
dvisc	0.0002304	Pa×s	547.33	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R30353&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume