Ethyl «alpha»-bromoheptanoate

Other names:	Heptanoic acid, 2-bromo-, ethyl ester
	ethyl 2-bromoheptanoate
Inchi:	InChI=1S/C9H17BrO2/c1-3-5-6-7-8(10)9(11)12-4-2/h8H,3-7H2,1-2H3
InchiKey:	GNCLPIAYAPQPOU-UHFFFAOYSA-N
Formula:	C9H17BrO2
SMILES:	CCCCCC(Br)C(=O)OCC
Mol. weight [g/mol]:	237.13
CAS:	5333-88-0

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	-3.00		Crippen Method
logp	2.893		Crippen Method
mcvol	162.610	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
rinpol	1282.00		NIST Webbook
rinpol	1382.00		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	425.81	J/mol×K	706.74	Joback Method
cpg	415.02	J/mol×K	674.86	Joback Method
cpg	403.67	J/mol×K	642.98	Joback Method
cpg	391.74	J/mol×K	611.09	Joback Method

cpg	379.22	J/mol×K	579.21	Joback Method
cpg	436.04	J/mol×K	738.62	Joback Method
dvisc	0.0002304	Pa×s	547.33	Joback Method
dvisc	0.0003004	Pa×s	507.47	Joback Method
dvisc	0.0004099	Pa×s	467.60	Joback Method
dvisc	0.0005925	Pa×s	427.74	Joback Method
dvisc	0.0009238	Pa×s	387.88	Joback Method
dvisc	0.0015948	Pa×s	348.01	Joback Method
dvisc	0.0031707	Pa×s	308.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5333880&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

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