Ethyl 2-bromooctanoate

Other names:	Octanoic acid, 2-bromo-, ethyl ester
Inchi:	InChI=1S/C10H19BrO2/c1-3-5-6-7-8-9(11)10(12)13-4-2/h9H,3-8H2,1-2H3
InchiKey:	JIQJOKSCSVMZAN-UHFFFAOYSA-N
Formula:	C10H19BrO2
SMILES:	CCCCCCC(Br)C(=O)OCC
Mol. weight [g/mol]:	251.16
CAS:	5445-29-4

Physical Properties

Property code	Value	Unit	Source
gf	-188.72	kJ/mol	Joback Method
hf	-473.48	kJ/mol	Joback Method
hfus	26.21	kJ/mol	Joback Method
hvap	53.06	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.283		Crippen Method
mcvol	176.700	ml/mol	McGowan Method
pc	2367.97	kPa	Joback Method
rinpol	1383.00		NIST Webbook
rinpol	1383.00		NIST Webbook
tb	570.21	K	Joback Method
tc	759.20	K	Joback Method
tf	319.42	K	Joback Method
vc	0.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.36	J/mol×K	570.21	Joback Method
cpg	476.60	J/mol×K	727.70	Joback Method
cpg	465.18	J/mol×K	696.20	Joback Method
cpg	453.16	J/mol×K	664.71	Joback Method
cpg	440.53	J/mol×K	633.21	Joback Method
cpg	427.26	J/mol×K	601.71	Joback Method

cpg	487.43	J/mol×K	759.20	Joback Method
dvisc	0.0002060	Pa×s	570.21	Joback Method
dvisc	0.0002698	Pa×s	528.41	Joback Method
dvisc	0.0003699	Pa×s	486.61	Joback Method
dvisc	0.0005384	Pa×s	444.82	Joback Method
dvisc	0.0008469	Pa×s	403.02	Joback Method
dvisc	0.0014794	Pa×s	361.22	Joback Method
dvisc	0.0029907	Pa×s	319.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5445294&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

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