Ethyl 2-bromodecanoate

Other names: Ethyl 2-bromodecanoate
Inchi: InChI=1S/C12H23BrO2/c1-3-5-6-7-8-9-10-11(13)12(14)15-4-2/h11H,3-10H2,1-2H3
InchiKey: IOOXHTJCOQWOJW-UHFFFAOYSA-N
Formula: C12H23BrO2
SMILES: CCCCCCCCC(Br)C(=O)OCC
Mol. weight [g/mol]: 279.22

Physical Properties

Property code	Value	Unit	Source
af	0.6974		Cheméo Relay (1.0)
hf	-590.66	kJ/mol	Cheméo Relay (1.0)
hfus	31.39	kJ/mol	Joback Method
hvap	73.49	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.78		Cheméo Relay (1.0)
logp	4.064		Crippen Method
mcvol	204.880	ml/mol	McGowan Method
pc	1980.59	kPa	Joback Method
rinpol	1682.00		NIST Webbook
rinpol	1587.00		NIST Webbook
rinpol	1682.00		NIST Webbook
tb	538.22	K	Cheméo Relay (1.0)
tc	719.22	K	Cheméo Relay (1.0)
tf	274.72	K	Cheméo Relay (1.0)
vc	0.760	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	512.85	J/mol×K	615.97	Joback Method
cpg	528.06	J/mol×K	646.81	Joback Method
cpg	542.55	J/mol×K	677.64	Joback Method
cpg	556.34	J/mol×K	708.48	Joback Method
cpg	569.46	J/mol×K	739.31	Joback Method
cpg	581.90	J/mol×K	770.15	Joback Method

cpg	593.71	J/mol×K	800.98	Joback Method
dvisc	0.0025939	Pa×s	341.96	Joback Method
dvisc	0.0012447	Pa×s	387.63	Joback Method
dvisc	0.0006973	Pa×s	433.30	Joback Method
dvisc	0.0004362	Pa×s	478.96	Joback Method
dvisc	0.0002961	Pa×s	524.63	Joback Method
dvisc	0.0002139	Pa×s	570.30	Joback Method
dvisc	0.0001621	Pa×s	615.97	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6974852&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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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