METHYL 3-BROMO-2,2-DICHLORO-PROPANOATE

Inchi: InChI=1S/C4H5BrCl2O2/c1-9-3(8)4(6,7)2-5/h2H2,1H3
InchiKey: AUHZFXMFSGANDP-UHFFFAOYSA-N
Formula: C4H5BrCl2O2
SMILES: COC(=O)C(Cl)(Cl)CBr
Mol. weight [g/mol]: 235.89

Physical Properties

Property code	Value	Unit	Source
hf	-432.61	kJ/mol	Cheméo Relay (1.0)
hfus	15.17	kJ/mol	Joback Method
hvap	57.57	kJ/mol	Cheméo Relay (1.0)
ie	10.62	eV	Cheméo Relay (1.0)
logp	1.728		Crippen Method
mcvol	116.640	ml/mol	McGowan Method
tb	471.83	K	Cheméo Relay (1.0)
tf	266.83	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	202.73	J/mol×K	505.00	Joback Method
cpg	236.94	J/mol×K	730.08	Joback Method
cpg	232.38	J/mol×K	692.57	Joback Method
cpg	227.40	J/mol×K	655.06	Joback Method
cpg	221.98	J/mol×K	617.54	Joback Method
cpg	216.08	J/mol×K	580.03	Joback Method
cpg	209.68	J/mol×K	542.51	Joback Method
dvisc	0.0007930	Pa×s	417.03	Joback Method
dvisc	0.0003551	Pa×s	505.00	Joback Method
dvisc	0.0004491	Pa×s	475.68	Joback Method
dvisc	0.0005857	Pa×s	446.35	Joback Method
dvisc	0.0027211	Pa×s	329.06	Joback Method
dvisc	0.0011240	Pa×s	387.71	Joback Method
dvisc	0.0016867	Pa×s	358.38	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C89294735&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

Legend

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
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point