

2-Bromopropionic acid, 3,5-dimethylphenyl ester

Inchi:	InChI=1S/C11H13BrO2/c1-7-4-8(2)6-10(5-7)14-11(13)9(3)12/h4-6,9H,1-3H3
InchiKey:	CJYJSYHSFIMPEF-UHFFFAOYSA-N
Formula:	C11H13BrO2
SMILES:	Cc1cc(C)cc(OC(=O)C(C)Br)c1
Mol. weight [g/mol]:	257.12

Physical Properties

Property code	Value	Unit	Source
gf	-87.15	kJ/mol	Joback Method
hf	-280.53	kJ/mol	Joback Method
hfus	22.06	kJ/mol	Joback Method
hvap	58.88	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	2.992		Crippen Method
mcvol	167.030	ml/mol	McGowan Method
pc	2921.84	kPa	Joback Method
rinpol	1551.00		NIST Webbook
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tb	629.73	K	Joback Method
tc	858.24	K	Joback Method
tf	382.15	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.22	J/molxK	629.73	Joback Method
cpg	397.38	J/molxK	667.81	Joback Method
cpg	409.71	J/molxK	705.90	Joback Method
cpg	421.24	J/molxK	743.98	Joback Method
cpg	431.97	J/molxK	782.07	Joback Method
cpg	441.95	J/molxK	820.15	Joback Method
cpg	451.17	J/molxK	858.24	Joback Method
dvisc	0.0013379	Paxs	382.15	Joback Method

dvisc	0.0008100	Paxs	423.41	Joback Method
dvisc	0.0005361	Paxs	464.68	Joback Method
dvisc	0.0003795	Paxs	505.94	Joback Method
dvisc	0.0002830	Paxs	547.20	Joback Method
dvisc	0.0002199	Paxs	588.47	Joback Method
dvisc	0.0001767	Paxs	629.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308024&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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