BUTANOIC ACID, 2-BROMO-, PENTYL ESTER

Other names: Pentyl 2-bromobutanoate
Inchi: InChI=1S/C9H17BrO2/c1-3-5-6-7-12-9(11)8(10)4-2/h8H,3-7H2,1-2H3
InchiKey: TYNCRXMYKJONLT-UHFFFAOYSA-N
Formula: C9H17BrO2
SMILES: CCCCCOC(=O)C(Br)CC
Mol. weight [g/mol]: 237.14

Physical Properties

Property code	Value	Unit	Source
af	0.6084		Cheméo Relay (1.0)
hf	-539.06	kJ/mol	Cheméo Relay (1.0)
hfus	23.62	kJ/mol	Joback Method
hvap	59.40	kJ/mol	Cheméo Relay (1.0)
ie	9.77	eV	Cheméo Relay (1.0)
log10ws	-3.25		Cheméo Relay (1.0)
logp	2.893		Crippen Method
mcvol	162.610	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
rinpol	1279.00		NIST Webbook
rinpol	1279.00		NIST Webbook
tb	493.27	K	Cheméo Relay (1.0)
tc	683.75	K	Cheméo Relay (1.0)
tf	252.59	K	Cheméo Relay (1.0)
vc	0.593	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.10	J/mol×K	547.33	Joback Method
cpg	436.04	J/mol×K	738.62	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
dvisc	0.0005925	Pa×s	427.74	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	0.0031707	Pa×s	308.15	Joback Method
dvisc	0.0009238	Pa×s	387.88	Joback Method
dvisc	0.0015948	Pa×s	348.01	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U131818&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
ie:	Ionization energy
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