

4-Penten-1-ol, dibromoacetate

Inchi:	InChI=1S/C7H10Br2O2/c1-2-3-4-5-11-7(10)6(8)9/h2,6H,1,3-5H2
InchiKey:	RGOU CZGJJDKQPF-UHFFFAOYSA-N
Formula:	C7H10Br2O2
SMILES:	C=CCCCOC(=O)C(Br)Br
Mol. weight [g/mol]:	285.96

Physical Properties

Property code	Value	Unit	Source
gf	-111.82	kJ/mol	Joback Method
hf	-259.80	kJ/mol	Joback Method
hfus	22.44	kJ/mol	Joback Method
hvap	52.14	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.612		Crippen Method
mvol	147.630	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
rinpol	1318.00		NIST Webbook
ripol	1928.00		NIST Webbook
tb	564.41	K	Joback Method
tc	779.02	K	Joback Method
tf	343.65	K	Joback Method
vc	0.550	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.83	J/molxK	564.41	Joback Method
cpg	336.16	J/molxK	743.25	Joback Method
cpg	328.56	J/molxK	707.48	Joback Method
cpg	320.45	J/molxK	671.72	Joback Method
cpg	311.81	J/molxK	635.95	Joback Method
cpg	302.61	J/molxK	600.18	Joback Method
cpg	343.28	J/molxK	779.02	Joback Method
dvisc	0.0002697	Paxs	564.41	Joback Method

dvisc	0.0003402	Paxs	527.62	Joback Method
dvisc	0.0004444	Paxs	490.82	Joback Method
dvisc	0.0006062	Paxs	454.03	Joback Method
dvisc	0.0008734	Paxs	417.24	Joback Method
dvisc	0.0013504	Paxs	380.44	Joback Method
dvisc	0.0022921	Paxs	343.65	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R26489&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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