Cumyl bromide

Inchi: InChI=1S/C9H11Br/c1-9(2,10)8-6-4-3-5-7-8/h3-7H,1-2H3
InchiKey: WSFSJXBURLJOFD-UHFFFAOYSA-N
Formula: C9H11Br
SMILES: CC(C)(Br)c1ccccc1
Mol. weight [g/mol]: 199.09

Physical Properties

Property code	Value	Unit	Source
gf	154.47	kJ/mol	Joback Method
hf	25.02	kJ/mol	Joback Method
hfus	10.98	kJ/mol	Joback Method
hvap	43.04	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.317		Crippen Method
mcvol	131.410	ml/mol	McGowan Method
pc	3615.89	kPa	Joback Method
rinpol	1181.00		NIST Webbook
tb	494.93	K	Joback Method
tc	735.23	K	Joback Method
tf	279.83	K	Joback Method
vc	0.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.96	J/mol×K	494.93	Joback Method
cpg	319.41	J/mol×K	695.18	Joback Method
cpg	309.17	J/mol×K	655.13	Joback Method
cpg	298.00	J/mol×K	615.08	Joback Method
cpg	285.80	J/mol×K	575.03	Joback Method
cpg	272.48	J/mol×K	534.98	Joback Method
cpg	328.79	J/mol×K	735.23	Joback Method
dvisc	0.0002728	Pa×s	494.93	Joback Method
dvisc	0.0003576	Pa×s	459.08	Joback Method

dvisc	0.0004909	Pa×s	423.23	Joback Method
dvisc	0.0007145	Pa×s	387.38	Joback Method
dvisc	0.0011228	Pa×s	351.53	Joback Method
dvisc	0.0019550	Pa×s	315.68	Joback Method
dvisc	0.0039237	Pa×s	279.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R558897&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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