

Cumyl iodide

Inchi:	InChI=1S/C9H11I/c1-9(2,10)8-6-4-3-5-7-8/h3-7H,1-2H3
InchiKey:	NRUOAXAWGSOGNL-UHFFFAOYSA-N
Formula:	C9H11I
SMILES:	CC(C)(I)c1ccccc1
Mol. weight [g/mol]:	246.09

Physical Properties

Property code	Value	Unit	Source
gf	198.27	kJ/mol	Joback Method
hf	75.56	kJ/mol	Joback Method
hfus	10.10	kJ/mol	Joback Method
hvap	45.98	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.357		Crippen Method
mcvol	139.730	ml/mol	McGowan Method
pc	3250.43	kPa	Joback Method
rinpol	1294.00		NIST Webbook
rinpol	1294.00		NIST Webbook
tb	521.91	K	Joback Method
tc	781.07	K	Joback Method
tf	278.09	K	Joback Method
vc	0.508	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.89	J/molxK	521.91	Joback Method
cpg	284.41	J/molxK	565.10	Joback Method
cpg	297.60	J/molxK	608.30	Joback Method
cpg	309.58	J/molxK	651.49	Joback Method
cpg	320.46	J/molxK	694.69	Joback Method
cpg	330.35	J/molxK	737.88	Joback Method
cpg	339.38	J/molxK	781.07	Joback Method
dvisc	0.0053944	Paxs	278.09	Joback Method

dvisc	0.0023773	Paxs	318.73	Joback Method
dvisc	0.0012609	Paxs	359.36	Joback Method
dvisc	0.0007608	Paxs	400.00	Joback Method
dvisc	0.0005039	Paxs	440.64	Joback Method
dvisc	0.0003577	Paxs	481.27	Joback Method
dvisc	0.0002679	Paxs	521.91	Joback Method

Sources

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=R558911&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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