

ALPHA-BROMO-PARA-TOLUNITRILE

Other names:	4-Cyanobenzyl bromide 4-(Bromomethyl)benzonitrile Benzonitrile, 4-(bromomethyl)- p-(Bromomethyl)benzonitrile p-Cyanobenzyl bromide p-Tolunitrile, «alpha»-bromo- p-Toluonitrile, «alpha»-bromo- Benzonitrile, p-(bromomethyl)- NSC 95792 «alpha»-bromo-p-toluonitrile
Inchi:	InChI=1S/C8H6BrN/c9-5-7-1-3-8(6-10)4-2-7/h1-4H,5H2
InchiKey:	UMLFTCYAQPPZER-UHFFFAOYSA-N
Formula:	C8H6BrN
SMILES:	N#Cc1ccc(CBr)cc1
Mol. weight [g/mol]:	196.05

Physical Properties

Property code	Value	Unit	Source
af	0.5075		Cheméo Relay (1.0)
gf	266.76	kJ/mol	Joback Method
hf	193.00	kJ/mol	Cheméo Relay (1.0)
hfus	16.92	kJ/mol	Joback Method
hvap	70.89	kJ/mol	Cheméo Relay (1.0)
ie	9.70	eV	Cheméo Relay (1.0)
log10ws	-2.89		Cheméo Relay (1.0)
logp	2.453		Crippen Method
mcvol	118.700	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
tb	539.88	K	Cheméo Relay (1.0)
tc	782.72	K	Cheméo Relay (1.0)
tf	374.03	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.81	J/mol×K	582.34	Joback Method
cpg	239.86	J/mol×K	623.60	Joback Method
cpg	248.22	J/mol×K	664.87	Joback Method
cpg	255.92	J/mol×K	706.13	Joback Method
cpg	263.01	J/mol×K	747.39	Joback Method
cpg	269.55	J/mol×K	788.66	Joback Method
cpg	275.58	J/mol×K	829.92	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C17201433&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

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

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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