

BUTYL CYANOACETATE

Other names:	Butyl cyanoacetate Cyanoacetic acid n-butyl ester Acetic acid, cyano-, butyl ester
Inchi:	InChI=1S/C7H11NO2/c1-2-3-6-10-7(9)4-5-8/h2-4,6H2,1H3
InchiKey:	DJACTCNGCHPGOI-UHFFFAOYSA-N
Formula:	C7H11NO2
SMILES:	CCCCOC(=O)CC#N
Mol. weight [g/mol]:	141.17

Physical Properties

Property code	Value	Unit	Source
af	0.5786		Cheméo Relay (1.0)
hf	-325.64	kJ/mol	Cheméo Relay (1.0)
hfus	18.18	kJ/mol	Joback Method
hvap	67.60	kJ/mol	Cheméo Relay (1.0)
ie	10.51	eV	Cheméo Relay (1.0)
log10ws	-1.31		Cheméo Relay (1.0)
logp	1.243		Crippen Method
mcvol	118.310	ml/mol	McGowan Method
pc	2862.74	kPa	Joback Method
tb	504.19	K	Cheméo Relay (1.0)
tc	671.23	K	Cheméo Relay (1.0)
tf	287.43	K	Cheméo Relay (1.0)
vc	0.441	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.53	J/mol×K	537.93	Joback Method
cpg	275.19	J/mol×K	570.48	Joback Method
cpg	284.44	J/mol×K	603.03	Joback Method
cpg	293.28	J/mol×K	635.59	Joback Method
cpg	301.71	J/mol×K	668.14	Joback Method
cpg	309.73	J/mol×K	700.69	Joback Method

cpg

317.35

J/mol×K

733.24

Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	388.20	K	2.00	NIST Webbook

Sources

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5459585&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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