2-Butanone, 4-(diethylamino)-

Other names: 1-(Diethylamino)-3-butanone
4-(Diethylamino)-2-butanone
4-(N,N-Diethylamino)butan-2-one
4-(diethylamino)butan-2-one
Inchi: InChI=1S/C8H17NO/c1-4-9(5-2)7-6-8(3)10/h4-7H2,1-3H3
InchiKey: XLEOCTUCGZANAC-UHFFFAOYSA-N
Formula: C8H17NO
SMILES: CCN(CC)CCC(C)=O
Mol. weight [g/mol]: 143.23
CAS: 3299-38-5

Physical Properties

Property code	Value	Unit	Source
gf	-1.66	kJ/mol	Joback Method
hf	-253.50	kJ/mol	Joback Method
hfus	21.10	kJ/mol	Joback Method
hvap	42.19	kJ/mol	Joback Method
log10ws	-1.02		Crippen Method
logp	1.307		Crippen Method
mcvol	135.130	ml/mol	McGowan Method
pc	2698.60	kPa	Joback Method
rinpol	1025.00		NIST Webbook
rinpol	1025.00		NIST Webbook
rinpol	1025.00		NIST Webbook
tb	448.75	K	Joback Method
tc	622.49	K	Joback Method
tf	262.32	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.50	J/mol×K	448.75	Joback Method
cpg	299.93	J/mol×K	477.71	Joback Method

cpg	312.79	J/mol×K	506.66	Joback Method
cpg	325.09	J/mol×K	535.62	Joback Method
cpg	336.84	J/mol×K	564.58	Joback Method
cpg	348.07	J/mol×K	593.54	Joback Method
cpg	358.78	J/mol×K	622.49	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	350.20	K	2.10	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3299385&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

Legend

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
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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume