

Methoxyacetamide, N-heptyl-N-octyl-

Inchi:	InChI=1S/C18H37NO2/c1-4-6-8-10-12-14-16-19(18(20)17-21-3)15-13-11-9-7-5-2/h4-17H
InchiKey:	JDPDRTDNKMSUAA-UHFFFAOYSA-N
Formula:	C18H37NO2
SMILES:	CCCCCCCCN(CCCCCC)C(=O)COC
Mol. weight [g/mol]:	299.49

Physical Properties

Property code	Value	Unit	Source
gf	-22.46	kJ/mol	Joback Method
hf	-592.12	kJ/mol	Joback Method
hfus	48.18	kJ/mol	Joback Method
hvap	66.86	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.792		Crippen Method
mvol	281.900	ml/mol	McGowan Method
pc	1187.42	kPa	Joback Method
rinpol	2140.00		NIST Webbook
rinpol	2140.00		NIST Webbook
tb	699.97	K	Joback Method
tc	868.44	K	Joback Method
tf	397.25	K	Joback Method
vc	1.085	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	832.06	J/mol×K	699.97	Joback Method
cpg	851.06	J/mol×K	728.05	Joback Method
cpg	869.19	J/mol×K	756.13	Joback Method
cpg	886.47	J/mol×K	784.20	Joback Method
cpg	902.93	J/mol×K	812.28	Joback Method
cpg	918.58	J/mol×K	840.36	Joback Method
cpg	933.46	J/mol×K	868.44	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=U308495&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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