

Acetoxyacetamide, N,N-bis(2-ethylhexyl)-

Inchi: InChI=1S/C20H39NO3/c1-6-10-12-18(8-3)14-21(20(23)16-24-17(5)22)15-19(9-4)13-11-7
InchiKey: XWBXBJSHUDNSPL-UHFFFAOYSA-N
Formula: C20H39NO3
SMILES: CCCCC(CC)CN(CC(CC)CCCC)C(=O)COC(C)=O
Mol. weight [g/mol]: 341.53

Physical Properties

Property code	Value	Unit	Source
gf	-139.42	kJ/mol	Joback Method
hf	-756.54	kJ/mol	Joback Method
hfus	47.92	kJ/mol	Joback Method
hvap	77.28	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.811		Crippen Method
mcvol	311.650	ml/mol	McGowan Method
pc	1100.08	kPa	Joback Method
rinpol	2150.00		NIST Webbook
tb	798.72	K	Joback Method
tc	982.42	K	Joback Method
tf	439.72	K	Joback Method
vc	1.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	981.56	J/mol×K	798.72	Joback Method
cpg	1000.36	J/mol×K	829.34	Joback Method
cpg	1018.11	J/mol×K	859.95	Joback Method
cpg	1034.83	J/mol×K	890.57	Joback Method
cpg	1050.58	J/mol×K	921.19	Joback Method
cpg	1065.37	J/mol×K	951.80	Joback Method
cpg	1079.23	J/mol×K	982.42	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=U308295&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
hvac:	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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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