Allyldiethylacetamide

Other names:	4-Pentenamide, 2,2-diethyl-
	Diethylallylacetamide
	Epinoval
	Novonal
	2,2-Diethyl-4-pentenamide
	Allyldiethylacetamide
Inchi:	InChI=1S/C9H17NO/c1-4-7-9(5-2,6-3)8(10)11/h4H,1,5-7H2,2-3H3,(H2,10,11)
InchiKey:	LOMDVEFCNVDZMZ-UHFFFAOYSA-N
Formula:	C9H17NO
SMILES:	C=CCC(CC)(CC)C(N)=O
Mol. weight [g/mol]:	155.24

Physical Properties

Property code	Value	Unit	Source
hfus	17.17	kJ/mol	Joback Method
hvap	57.12	kJ/mol	Cheméo Relay (1.0)
logp	1.854		Crippen Method
mcvol	144.920	ml/mol	McGowan Method
rinpol	1285.00		NIST Webbook
rinpol	1285.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.62	J/mol×K	525.17	Joback Method
cpg	357.66	J/mol×K	558.51	Joback Method
cpg	370.87	J/mol×K	591.86	Joback Method
cpg	383.29	J/mol×K	625.20	Joback Method
cpg	394.97	J/mol×K	658.54	Joback Method
cpg	405.95	J/mol×K	691.88	Joback Method
cpg	416.27	J/mol×K	725.23	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C512481&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

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices