N-(2-Methylbutyl)-(2E,6Z,8E)-decatrienamide

Inchi: InChI=1S/C15H25NO/c1-4-6-7-8-9-10-11-12-15(17)16-13-14(3)5-2/h4,6-8,11-12,14H,5,9
InchiKey: LWJDBUUOYULAFU-KVSSZBNBSA-N
Formula: C15H25NO
SMILES: CC=CC=CCCC=CC(=O)NCC(C)CC
Mol. weight [g/mol]: 235.37

Physical Properties

Property code	Value	Unit	Source
gf	274.11	kJ/mol	Joback Method
hf	-65.66	kJ/mol	Joback Method
hfus	38.39	kJ/mol	Joback Method
hvap	61.65	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.617		Crippen Method
mcvol	220.860	ml/mol	McGowan Method
pc	1710.36	kPa	Joback Method
rinpol	1946.00		NIST Webbook
ripol	2546.00		NIST Webbook
tb	658.68	K	Joback Method
tc	849.39	K	Joback Method
tf	331.16	K	Joback Method
vc	0.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.08	J/mol×K	658.68	Joback Method
cpg	605.42	J/mol×K	690.46	Joback Method
cpg	620.89	J/mol×K	722.25	Joback Method
cpg	635.54	J/mol×K	754.03	Joback Method
cpg	649.44	J/mol×K	785.82	Joback Method
cpg	662.64	J/mol×K	817.60	Joback Method
cpg	675.20	J/mol×K	849.39	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=U106160&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume