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

Inchi: InChI=1S/C14H23NO/c1-4-5-6-7-8-9-10-11-14(16)15-12-13(2)3/h4-7,10-11,13H,8-9,12H
InchiKey: BXOCHUWSGYYSFW-HVWOQQCMSA-N
Formula: C14H23NO
SMILES: CC=CC=CCCC=CC(=O)NCC(C)C
Mol. weight [g/mol]: 221.34

Physical Properties

Property code	Value	Unit	Source
gf	265.69	kJ/mol	Joback Method
hf	-45.02	kJ/mol	Joback Method
hfus	35.80	kJ/mol	Joback Method
hvap	59.43	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.227		Crippen Method
mcvol	206.770	ml/mol	McGowan Method
pc	1854.71	kPa	Joback Method
rinpol	1844.00		NIST Webbook
tb	635.80	K	Joback Method
tc	828.48	K	Joback Method
tf	319.89	K	Joback Method
vc	0.794	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.17	J/mol×K	635.80	Joback Method
cpg	552.10	J/mol×K	667.91	Joback Method
cpg	567.15	J/mol×K	700.03	Joback Method
cpg	581.38	J/mol×K	732.14	Joback Method
cpg	594.86	J/mol×K	764.25	Joback Method
cpg	607.64	J/mol×K	796.36	Joback Method
cpg	619.78	J/mol×K	828.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U106175&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume