2,4,9-Octadecatrienoyl isobutylamide

Inchi: InChI=1S/C22H39NO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22(24)23-20-21(2)
InchiKey: QHGVDYOXPZHMLH-NWAKFNDOSA-N
Formula: C22H39NO
SMILES: CCCCCCCCC=CCCCC=CC=CC(=O)NCC(C)C
Mol. weight [g/mol]: 333.55

Physical Properties

Property code	Value	Unit	Source
gf	333.05	kJ/mol	Joback Method
hf	-210.14	kJ/mol	Joback Method
hfus	56.52	kJ/mol	Joback Method
hvap	77.23	kJ/mol	Joback Method
log10ws	-7.32		Crippen Method
logp	6.348		Crippen Method
mcvol	319.490	ml/mol	McGowan Method
pc	1047.33	kPa	Joback Method
rinpol	2738.00		NIST Webbook
tb	818.84	K	Joback Method
tc	1008.72	K	Joback Method
tf	410.05	K	Joback Method
vc	1.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	991.71	J/mol×K	818.84	Joback Method
cpg	1010.63	J/mol×K	850.49	Joback Method
cpg	1028.65	J/mol×K	882.13	Joback Method
cpg	1045.84	J/mol×K	913.78	Joback Method
cpg	1062.26	J/mol×K	945.42	Joback Method
cpg	1078.01	J/mol×K	977.07	Joback Method
cpg	1093.14	J/mol×K	1008.72	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=R545841&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume