2,4-Hexadecadienoyl isobutyramide

Inchi: InChI=1S/C10H17NO/c1-4-5-6-7-10(12)11-8-9(2)3/h4-7,9H,8H2,1-3H3,(H,11,12)/b5-4+,7

InchiKey: DHXYPSWRPDLKGG-YTXTXJHMSA-N

Formula: C10H17NO

SMILES: CC=CC=CC(=O)NCC(C)C

Mol. weight [g/mol]: 167.25

Physical Properties

Property code	Value	Unit	Source
gf	151.79	kJ/mol	Joback Method
hf	-79.68	kJ/mol	Joback Method
hfus	25.24	kJ/mol	Joback Method
hvap	50.56	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	1.891		Crippen Method
mcvol	154.710	ml/mol	McGowan Method
pc	2525.19	kPa	Joback Method
rinpol	2557.00		NIST Webbook
rinpol	2557.00		NIST Webbook
tb	540.12	K	Joback Method
tc	734.73	K	Joback Method
tf	279.89	K	Joback Method
vc	0.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.69	J/mol×K	540.12	Joback Method
cpg	371.80	J/mol×K	572.56	Joback Method
cpg	385.12	J/mol×K	604.99	Joback Method
cpg	397.71	J/mol×K	637.43	Joback Method
cpg	409.60	J/mol×K	669.86	Joback Method
cpg	420.83	J/mol×K	702.30	Joback Method
cpg	431.44	J/mol×K	734.73	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R545910&Units=SI

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