N,n-diphenyl isobutyramide

Inchi: InChI=1S/C16H17NO/c1-13(2)16(18)17(14-9-5-3-6-10-14)15-11-7-4-8-12-15/h3-13H,1-2
InchiKey: MCHBSCOEBHAUDR-UHFFFAOYSA-N
Formula: C16H17NO
SMILES: CC(C)C(=O)N(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 239.31
CAS: 69737-54-8

Physical Properties

Property code	Value	Unit	Source
gf	288.08	kJ/mol	Joback Method
hf	49.16	kJ/mol	Joback Method
hfus	26.38	kJ/mol	Joback Method
hvap	64.16	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	4.007		Crippen Method
mcvol	200.330	ml/mol	McGowan Method
pc	2443.48	kPa	Joback Method
tb	684.71	K	Joback Method
tc	922.04	K	Joback Method
tf	390.32	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.72	J/mol×K	684.71	Joback Method
cpg	548.91	J/mol×K	724.26	Joback Method
cpg	564.70	J/mol×K	763.82	Joback Method
cpg	579.20	J/mol×K	803.37	Joback Method
cpg	592.50	J/mol×K	842.93	Joback Method
cpg	604.69	J/mol×K	882.48	Joback Method
cpg	615.87	J/mol×K	922.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C69737548&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume