Undec-10-ynoic acid, isobutyl ester

Inchi: InChI=1S/C15H26O2/c1-4-5-6-7-8-9-10-11-12-15(16)17-13-14(2)3/h1,14H,5-13H2,2-3H3
InchiKey: KDUWBXGOYJXAPO-UHFFFAOYSA-N
Formula: C15H26O2
SMILES: C#CCCCCCCCCC(=O)OCC(C)C
Mol. weight [g/mol]: 238.37

Physical Properties

Property code	Value	Unit	Source
gf	62.13	kJ/mol	Joback Method
hf	-311.11	kJ/mol	Joback Method
hfus	36.84	kJ/mol	Joback Method
hvap	57.61	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.940		Crippen Method
mcvol	221.050	ml/mol	McGowan Method
pc	1657.84	kPa	Joback Method
rinpol	1676.00		NIST Webbook
tb	608.57	K	Joback Method
tc	786.86	K	Joback Method
tf	362.94	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.01	J/mol×K	608.57	Joback Method
cpg	593.84	J/mol×K	638.28	Joback Method
cpg	609.90	J/mol×K	668.00	Joback Method
cpg	625.23	J/mol×K	697.71	Joback Method
cpg	639.84	J/mol×K	727.43	Joback Method
cpg	653.75	J/mol×K	757.14	Joback Method
cpg	666.97	J/mol×K	786.86	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=U406156&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

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