Undec-10-ynoic acid, butyl ester

Inchi: InChI=1S/C15H26O2/c1-3-5-7-8-9-10-11-12-13-15(16)17-14-6-4-2/h1H,4-14H2,2H3
InchiKey: GDIRFVXFPCQNDO-UHFFFAOYSA-N
Formula: C15H26O2
SMILES: C#CCCCCCCCCC(=O)OCCCC
Mol. weight [g/mol]: 238.37

Physical Properties

Property code	Value	Unit	Source
gf	64.57	kJ/mol	Joback Method
hf	-305.83	kJ/mol	Joback Method
hfus	40.37	kJ/mol	Joback Method
hvap	58.00	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	4.084		Crippen Method
mcvol	221.050	ml/mol	McGowan Method
pc	1647.09	kPa	Joback Method
rinpol	1718.00		NIST Webbook
rinpol	1718.00		NIST Webbook
tb	609.01	K	Joback Method
tc	784.40	K	Joback Method
tf	377.94	K	Joback Method
vc	0.862	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.64	J/mol×K	609.01	Joback Method
cpg	593.15	J/mol×K	638.24	Joback Method
cpg	608.93	J/mol×K	667.47	Joback Method
cpg	624.00	J/mol×K	696.70	Joback Method
cpg	638.38	J/mol×K	725.93	Joback Method
cpg	652.09	J/mol×K	755.17	Joback Method
cpg	665.15	J/mol×K	784.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406157&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

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