

Butyric acid, 4-phenyl-, undec-2-en-1-yl ester

Inchi:	InChI=1S/C21H32O2/c1-2-3-4-5-6-7-8-9-13-19-23-21(22)18-14-17-20-15-11-10-12-16-20
InchiKey:	MTRLQWICLCBEJH-UKTHLTGXSA-N
Formula:	C21H32O2
SMILES:	CCCCCCCCC=CCOC(=O)CCCc1ccccc1
Mol. weight [g/mol]:	316.48

Physical Properties

Property code	Value	Unit	Source
gf	84.65	kJ/mol	Joback Method
hf	-367.82	kJ/mol	Joback Method
hfus	47.18	kJ/mol	Joback Method
hvap	73.73	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	5.859		Crippen Method
mvol	286.130	ml/mol	McGowan Method
pc	1270.97	kPa	Joback Method
rinpol	2396.00		NIST Webbook
rinpol	2396.00		NIST Webbook
tb	787.01	K	Joback Method
tc	982.19	K	Joback Method
tf	419.93	K	Joback Method
vc	1.107	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	860.57	J/molxK	787.01	Joback Method
cpg	878.62	J/molxK	819.54	Joback Method
cpg	895.62	J/molxK	852.07	Joback Method
cpg	911.63	J/molxK	884.60	Joback Method
cpg	926.69	J/molxK	917.13	Joback Method
cpg	940.86	J/molxK	949.66	Joback Method
cpg	954.19	J/molxK	982.19	Joback Method
dvisc	0.0010888	Paxs	419.93	Joback Method

dvisc	0.0004857	Paxs	481.11	Joback Method
dvisc	0.0002600	Paxs	542.29	Joback Method
dvisc	0.0001579	Paxs	603.47	Joback Method
dvisc	0.0001052	Paxs	664.65	Joback Method
dvisc	0.0000750	Paxs	725.83	Joback Method
dvisc	0.0000564	Paxs	787.01	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U406988&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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