

Butyric acid, 2-phenyl-, dodec-2-en-1-yl ester

Inchi:	InChI=1S/C22H34O2/c1-3-5-6-7-8-9-10-11-12-16-19-24-22(23)21(4-2)20-17-14-13-15-18
InchiKey:	OKASAXVDJXILIH-FOWTUZBSSA-N
Formula:	C22H34O2
SMILES:	CCCCCCCCC=CCOC(=O)C(CC)c1ccccc1
Mol. weight [g/mol]:	330.50

Physical Properties

Property code	Value	Unit	Source
gf	90.63	kJ/mol	Joback Method
hf	-393.74	kJ/mol	Joback Method
hfus	46.24	kJ/mol	Joback Method
hvap	75.57	kJ/mol	Joback Method
log10ws	-6.81		Crippen Method
logp	6.420		Crippen Method
mvol	300.220	ml/mol	McGowan Method
pc	1194.82	kPa	Joback Method
rinpol	2345.00		NIST Webbook
rinpol	2345.00		NIST Webbook
tb	809.45	K	Joback Method
tc	1006.73	K	Joback Method
tf	416.20	K	Joback Method
vc	1.157	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	920.54	J/molxK	809.45	Joback Method
cpg	939.00	J/molxK	842.33	Joback Method
cpg	956.37	J/molxK	875.21	Joback Method
cpg	972.69	J/molxK	908.09	Joback Method
cpg	988.03	J/molxK	940.97	Joback Method
cpg	1002.45	J/molxK	973.85	Joback Method
cpg	1015.98	J/molxK	1006.73	Joback Method
dvisc	0.0011847	Paxs	416.20	Joback Method

dvisc	0.0004747	Paxs	481.74	Joback Method
dvisc	0.0002368	Paxs	547.28	Joback Method
dvisc	0.0001371	Paxs	612.82	Joback Method
dvisc	0.0000882	Paxs	678.37	Joback Method
dvisc	0.0000613	Paxs	743.91	Joback Method
dvisc	0.0000452	Paxs	809.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406867&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
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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