

4-Oxo-4-phenylbutyric acid, undecyl ester

Inchi:	InChI=1S/C21H32O3/c1-2-3-4-5-6-7-8-9-13-18-24-21(23)17-16-20(22)19-14-11-10-12-15
InchiKey:	JRVCOCSYOGYPV-UHFFFAOYSA-N
Formula:	C21H32O3
SMILES:	CCCCCCCCCOC(=O)CCC(=O)c1ccccc1
Mol. weight [g/mol]:	332.48

Physical Properties

Property code	Value	Unit	Source
gf	-124.49	kJ/mol	Joback Method
hf	-597.62	kJ/mol	Joback Method
hfus	48.57	kJ/mol	Joback Method
hvap	80.52	kJ/mol	Joback Method
log10ws	-6.44		Crippen Method
logp	5.724		Crippen Method
mcvol	292.000	ml/mol	McGowan Method
pc	1280.99	kPa	Joback Method
rinsol	2614.00		NIST Webbook
tb	836.72	K	Joback Method
tc	1035.46	K	Joback Method
tf	474.94	K	Joback Method
vc	1.133	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	907.80	J/molxK	836.72	Joback Method
cpg	981.62	J/molxK	1002.34	Joback Method
cpg	968.89	J/molxK	969.22	Joback Method
cpg	955.19	J/molxK	936.09	Joback Method
cpg	940.47	J/molxK	902.97	Joback Method
cpg	924.69	J/molxK	869.84	Joback Method
cpg	993.41	J/molxK	1035.46	Joback Method
dvisc	0.0000627	Paxs	836.72	Joback Method
dvisc	0.0000823	Paxs	776.42	Joback Method

dvisc	0.0001131	Paxs	716.13	Joback Method
dvisc	0.0001649	Paxs	655.83	Joback Method
dvisc	0.0002595	Paxs	595.53	Joback Method
dvisc	0.0004521	Paxs	535.24	Joback Method
dvisc	0.0009071	Paxs	474.94	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=U405982&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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