

4-Oxo-4-phenylbutyric acid, tetradecyl ester

Inchi:	InChI=1S/C24H38O3/c1-2-3-4-5-6-7-8-9-10-11-12-16-21-27-24(26)20-19-23(25)22-17-14
InchiKey:	YOEZMNOCRCZZST-UHFFFAOYSA-N
Formula:	C24H38O3
SMILES:	CCCCCCCCCCCCCOC(=O)CCC(=O)c1ccccc1
Mol. weight [g/mol]:	374.56

Physical Properties

Property code	Value	Unit	Source
gf	-99.23	kJ/mol	Joback Method
hf	-659.54	kJ/mol	Joback Method
hfus	56.34	kJ/mol	Joback Method
hvap	87.20	kJ/mol	Joback Method
log10ws	-7.69		Crippen Method
logp	6.894		Crippen Method
mvol	334.270	ml/mol	McGowan Method
pc	1052.77	kPa	Joback Method
rinpol	2921.00		NIST Webbook
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tb	905.36	K	Joback Method
tc	1110.26	K	Joback Method
tf	508.75	K	Joback Method
vc	1.302	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1089.59	J/molxK	905.36	Joback Method
cpg	1107.24	J/molxK	939.51	Joback Method
cpg	1123.66	J/molxK	973.66	Joback Method
cpg	1138.91	J/molxK	1007.81	Joback Method
cpg	1153.05	J/molxK	1041.96	Joback Method
cpg	1166.13	J/molxK	1076.11	Joback Method
cpg	1178.20	J/molxK	1110.26	Joback Method
dvisc	0.0006500	Paxs	508.75	Joback Method

dvisc	0.0003140	Paxs	574.85	Joback Method
dvisc	0.0001763	Paxs	640.95	Joback Method
dvisc	0.0001103	Paxs	707.06	Joback Method
dvisc	0.0000747	Paxs	773.16	Joback Method
dvisc	0.0000538	Paxs	839.26	Joback Method
dvisc	0.0000407	Paxs	905.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405985&Units=SI
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

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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