

4-Oxo-4-phenylbutyric acid, tridecyl ester

Inchi:	InChI=1S/C23H36O3/c1-2-3-4-5-6-7-8-9-10-11-15-20-26-23(25)19-18-22(24)21-16-13-12
InchiKey:	OJVFWWBKOTVKAK-UHFFFAOYSA-N
Formula:	C23H36O3
SMILES:	CCCCCCCCCCCCOC(=O)CCC(=O)c1ccccc1
Mol. weight [g/mol]:	360.53

Physical Properties

Property code	Value	Unit	Source
gf	-107.65	kJ/mol	Joback Method
hf	-638.90	kJ/mol	Joback Method
hfus	53.75	kJ/mol	Joback Method
hvap	84.97	kJ/mol	Joback Method
log10ws	-7.27		Crippen Method
logp	6.504		Crippen Method
mvol	320.180	ml/mol	McGowan Method
pc	1121.55	kPa	Joback Method
rinpol	2820.00		NIST Webbook
rinpol	2820.00		NIST Webbook
tb	882.48	K	Joback Method
tc	1084.52	K	Joback Method
tf	497.48	K	Joback Method
vc	1.246	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1028.31	J/molxK	882.48	Joback Method
cpg	1103.90	J/molxK	1050.85	Joback Method
cpg	1090.94	J/molxK	1017.17	Joback Method
cpg	1076.95	J/molxK	983.50	Joback Method
cpg	1061.88	J/molxK	949.83	Joback Method
cpg	1045.69	J/molxK	916.15	Joback Method
cpg	1115.88	J/molxK	1084.52	Joback Method
dvisc	0.0000471	Paxs	882.48	Joback Method

dvisc	0.0000622	Paxs	818.31	Joback Method
dvisc	0.0000860	Paxs	754.15	Joback Method
dvisc	0.0001264	Paxs	689.98	Joback Method
dvisc	0.0002011	Paxs	625.81	Joback Method
dvisc	0.0003558	Paxs	561.65	Joback Method
dvisc	0.0007291	Paxs	497.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405984&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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