

4-Oxo-4-phenylbutyric acid, octadecyl ester

Inchi:	InChI=1S/C28H46O3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20-25-31-28(30)24-23-27
InchiKey:	UWDBGFVEELSFOH-UHFFFAOYSA-N
Formula:	C28H46O3
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)CCC(=O)c1ccccc1
Mol. weight [g/mol]:	430.66

Physical Properties

Property code	Value	Unit	Source
gf	-65.55	kJ/mol	Joback Method
hf	-742.10	kJ/mol	Joback Method
hfus	66.70	kJ/mol	Joback Method
hvap	96.10	kJ/mol	Joback Method
log10ws	-9.37		Crippen Method
logp	8.454		Crippen Method
mcvol	390.630	ml/mol	McGowan Method
pc	832.42	kPa	Joback Method
rinsol	3345.00		NIST Webbook
tb	996.88	K	Joback Method
tc	1222.71	K	Joback Method
tf	553.83	K	Joback Method
vc	1.526	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1340.24	J/molxK	996.88	Joback Method
cpg	1359.36	J/molxK	1034.52	Joback Method
cpg	1376.98	J/molxK	1072.16	Joback Method
cpg	1393.18	J/molxK	1109.80	Joback Method
cpg	1408.06	J/molxK	1147.44	Joback Method
cpg	1421.70	J/molxK	1185.08	Joback Method
cpg	1434.19	J/molxK	1222.71	Joback Method
dvisc	0.0003977	Paxs	553.83	Joback Method
dvisc	0.0001853	Paxs	627.67	Joback Method

dvisc	0.0001014	Paxs	701.51	Joback Method
dvisc	0.0000623	Paxs	775.36	Joback Method
dvisc	0.0000416	Paxs	849.20	Joback Method
dvisc	0.0000296	Paxs	923.04	Joback Method
dvisc	0.0000222	Paxs	996.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405989&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

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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