

4-Oxo-4-phenylbutyric acid, heptadecyl ester

Inchi: InChI=1S/C27H44O3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-24-30-27(29)23-22-26(28)
InchiKey: WPQLMCFXTSNXQM-UHFFFAOYSA-N
Formula: C27H44O3
SMILES: CCCCCCCCCCCCCCCCCOC(=O)CCC(=O)c1ccccc1
Mol. weight [g/mol]: 416.64

Physical Properties

Property code	Value	Unit	Source
gf	-73.97	kJ/mol	Joback Method
hf	-721.46	kJ/mol	Joback Method
hfus	64.11	kJ/mol	Joback Method
hvap	93.87	kJ/mol	Joback Method
log10ws	-8.95		Crippen Method
logp	8.064		Crippen Method
mcvol	376.540	ml/mol	McGowan Method
pc	880.52	kPa	Joback Method
rinsol	3240.00		NIST Webbook
tb	974.00	K	Joback Method
tc	1193.03	K	Joback Method
tf	542.56	K	Joback Method
vc	1.470	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1276.84	J/molxK	974.00	Joback Method
cpg	1295.53	J/molxK	1010.50	Joback Method
cpg	1312.79	J/molxK	1047.01	Joback Method
cpg	1328.72	J/molxK	1083.51	Joback Method
cpg	1343.38	J/molxK	1120.02	Joback Method
cpg	1356.86	J/molxK	1156.52	Joback Method
cpg	1369.23	J/molxK	1193.03	Joback Method
dvisc	0.0004516	Paxs	542.56	Joback Method
dvisc	0.0002123	Paxs	614.47	Joback Method

dvisc	0.0001169	Paxs	686.37	Joback Method
dvisc	0.0000720	Paxs	758.28	Joback Method
dvisc	0.0000483	Paxs	830.19	Joback Method
dvisc	0.0000345	Paxs	902.09	Joback Method
dvisc	0.0000259	Paxs	974.00	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=U405988&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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