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
rinpol	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	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0001169	Pa×s	686.37	Joback Method
dvisc	0.0000720	Pa×s	758.28	Joback Method
dvisc	0.0000483	Pa×s	830.19	Joback Method
dvisc	0.0000345	Pa×s	902.09	Joback Method
dvisc	0.0000259	Pa×s	974.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405988&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Latest version available from:
https://www.chemeo.com/cid/86-352-6/4-Oxo-4-phenylbutyric-acid-heptadecyl-ester.pdf
Generated by Cheméo on 2024-10-12 03:12:01.459713942 +0000 UTC m=+3283584.096683191.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.