Eicosanoic acid, phenylmethyl ester

Other names: Benzyl icosanoate
Inchi: InChI=1S/C27H46O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-24-27(28)29-25-26
InchiKey: MFBVDRDCUYGRCJ-UHFFFAOYSA-N
Formula: C27H46O2
SMILES: CCCCCCCCCCCCCCCCCCCC(=O)OCc1ccccc1
Mol. weight [g/mol]: 402.65
CAS: 77509-04-7

Physical Properties

Property code	Value	Unit	Source
gf	54.95	kJ/mol	Joback Method
hf	-608.88	kJ/mol	Joback Method
hfus	62.51	kJ/mol	Joback Method
hvap	87.13	kJ/mol	Joback Method
log10ws	-9.59		Crippen Method
logp	8.771		Crippen Method
mcvol	374.970	ml/mol	McGowan Method
pc	848.50	kPa	Joback Method
rinpol	3003.30		NIST Webbook
rinpol	3003.30		NIST Webbook
tb	920.13	K	Joback Method
tc	1126.50	K	Joback Method
tf	492.63	K	Joback Method
vc	1.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1256.14	J/mol×K	920.13	Joback Method
cpg	1276.46	J/mol×K	954.52	Joback Method
cpg	1295.44	J/mol×K	988.92	Joback Method
cpg	1313.14	J/mol×K	1023.31	Joback Method
cpg	1329.63	J/mol×K	1057.71	Joback Method
cpg	1344.97	J/mol×K	1092.10	Joback Method

cpg	1359.23	J/mol×K	1126.50	Joback Method
dvisc	0.0005922	Pa×s	492.63	Joback Method
dvisc	0.0002570	Pa×s	563.88	Joback Method
dvisc	0.0001345	Pa×s	635.13	Joback Method
dvisc	0.0000802	Pa×s	706.38	Joback Method
dvisc	0.0000526	Pa×s	777.63	Joback Method
dvisc	0.0000370	Pa×s	848.88	Joback Method
dvisc	0.0000275	Pa×s	920.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77509047&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

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