Hexanedioic acid, octyl phenylmethyl ester

Other names: benzyl octyl adipate
Inchi: InChI=1S/C21H32O4/c1-2-3-4-5-6-12-17-24-20(22)15-10-11-16-21(23)25-18-19-13-8-7-9
InchiKey: DECACTMEFWAFRE-UHFFFAOYSA-N
Formula: C21H32O4
SMILES: CCCCCCCCOC(=O)CCCCC(=O)OCc1ccccc1
Mol. weight [g/mol]: 348.48
CAS: 3089-55-2

Physical Properties

Property code	Value	Unit	Source
gf	-229.49	kJ/mol	Joback Method
hf	-729.84	kJ/mol	Joback Method
hfus	49.76	kJ/mol	Joback Method
hvap	82.93	kJ/mol	Joback Method
log10ws	-5.94		Crippen Method
logp	5.194		Crippen Method
mcvol	297.870	ml/mol	McGowan Method
pc	1265.55	kPa	Joback Method
rinpol	2521.00		NIST Webbook
rinpol	2521.00		NIST Webbook
tb	859.14	K	Joback Method
tc	1059.46	K	Joback Method
tf	497.17	K	Joback Method
vc	1.151	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	937.74	J/mol×K	859.14	Joback Method
cpg	1008.48	J/mol×K	1026.07	Joback Method
cpg	996.55	J/mol×K	992.69	Joback Method
cpg	983.54	J/mol×K	959.30	Joback Method
cpg	969.42	J/mol×K	925.91	Joback Method
cpg	954.16	J/mol×K	892.53	Joback Method

cpg	1019.36	J/mol×K	1059.46	Joback Method
dvisc	0.0000470	Pa×s	859.14	Joback Method
dvisc	0.0000614	Pa×s	798.81	Joback Method
dvisc	0.0000840	Pa×s	738.48	Joback Method
dvisc	0.0001214	Pa×s	678.15	Joback Method
dvisc	0.0001885	Pa×s	617.83	Joback Method
dvisc	0.0003221	Pa×s	557.50	Joback Method
dvisc	0.0006267	Pa×s	497.17	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3089552&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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