Hexadecanoic acid, phenylmethyl ester

Other names: Benzyl palmitate
Inchi: InChI=1S/C23H38O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-17-20-23(24)25-21-22-18-15-14-16
InchiKey: CKEVMZSLVHLLBF-UHFFFAOYSA-N
Formula: C23H38O2
SMILES: CCCCCCCCCCCCCCCC(=O)OCc1ccccc1
Mol. weight [g/mol]: 346.55
CAS: 41755-60-6

Physical Properties

Property code	Value	Unit	Source
gf	21.27	kJ/mol	Joback Method
hf	-526.32	kJ/mol	Joback Method
hfus	52.15	kJ/mol	Joback Method
hvap	78.22	kJ/mol	Joback Method
log10ws	-7.91		Crippen Method
logp	7.211		Crippen Method
mcvol	318.610	ml/mol	McGowan Method
pc	1075.69	kPa	Joback Method
rinpol	2527.00		NIST Webbook
rinpol	2527.00		NIST Webbook
rinpol	2587.80		NIST Webbook
rinpol	2587.80		NIST Webbook
tb	828.61	K	Joback Method
tc	1021.45	K	Joback Method
tf	447.55	K	Joback Method
vc	1.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1006.10	J/mol×K	828.61	Joback Method
cpg	1090.23	J/mol×K	989.31	Joback Method
cpg	1075.50	J/mol×K	957.17	Joback Method
cpg	1059.76	J/mol×K	925.03	Joback Method

cpg	1042.98	J/mol×K	892.89	Joback Method
cpg	1025.11	J/mol×K	860.75	Joback Method
cpg	1104.00	J/mol×K	1021.45	Joback Method
dvisc	0.0000492	Pa×s	828.61	Joback Method
dvisc	0.0000657	Pa×s	765.10	Joback Method
dvisc	0.0000923	Pa×s	701.59	Joback Method
dvisc	0.0001389	Pa×s	638.08	Joback Method
dvisc	0.0002287	Pa×s	574.57	Joback Method
dvisc	0.0004261	Pa×s	511.06	Joback Method
dvisc	0.0009474	Pa×s	447.55	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C41755606&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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