Phenethyl stearate

Inchi: InChI=1S/C26H44O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-22-26(27)28-24-23-25-20
InchiKey: NEPWYQKPLAOWOC-UHFFFAOYSA-N
Formula: C26H44O2
SMILES: CCCCCCCCCCCCCCCCCC(=O)OCCc1ccccc1
Mol. weight [g/mol]: 388.63
CAS: 72934-13-5

Physical Properties

Property code	Value	Unit	Source
gf	46.53	kJ/mol	Joback Method
hf	-588.24	kJ/mol	Joback Method
hfus	59.92	kJ/mol	Joback Method
hvap	84.90	kJ/mol	Joback Method
log10ws	-8.67		Crippen Method
logp	8.034		Crippen Method
mcvol	360.880	ml/mol	McGowan Method
pc	898.02	kPa	Joback Method
rinpol	2889.90		NIST Webbook
rinpol	2889.90		NIST Webbook
rinpol	2893.60		NIST Webbook
tb	897.25	K	Joback Method
tc	1098.93	K	Joback Method
tf	481.36	K	Joback Method
vc	1.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1192.71	J/mol×K	897.25	Joback Method
cpg	1280.17	J/mol×K	1065.31	Joback Method
cpg	1265.00	J/mol×K	1031.70	Joback Method
cpg	1248.73	J/mol×K	998.09	Joback Method
cpg	1231.30	J/mol×K	964.48	Joback Method
cpg	1212.65	J/mol×K	930.86	Joback Method

cpg	1294.30	J/mol×K	1098.93	Joback Method
dvisc	0.0000319	Pa×s	897.25	Joback Method
dvisc	0.0000429	Pa×s	827.93	Joback Method
dvisc	0.0000608	Pa×s	758.62	Joback Method
dvisc	0.0000924	Pa×s	689.30	Joback Method
dvisc	0.0001542	Pa×s	619.99	Joback Method
dvisc	0.0002930	Pa×s	550.67	Joback Method
dvisc	0.0006695	Pa×s	481.36	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C72934135&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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