phenethyl ester

Inchi: InChI=1S/C16H18O/c1-3-7-15(8-4-1)11-13-17-14-12-16-9-5-2-6-10-16/h1-10H,11-14H2
InchiKey: AMOYMEBHYUTMKJ-UHFFFAOYSA-N
Formula: C16H18O
SMILES: c1ccc(CCOCCc2ccccc2)cc1
Mol. weight [g/mol]: 226.31

Physical Properties

Property code	Value	Unit	Source
gf	203.66	kJ/mol	Joback Method
hf	-32.73	kJ/mol	Joback Method
hfus	26.47	kJ/mol	Joback Method
hvap	58.17	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.488		Crippen Method
mcvol	194.650	ml/mol	McGowan Method
pc	2248.26	kPa	Joback Method
rinpol	1502.00		NIST Webbook
tb	641.26	K	Joback Method
tc	868.11	K	Joback Method
tf	345.15	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.57	J/mol×K	641.26	Joback Method
cpg	578.01	J/mol×K	830.30	Joback Method
cpg	564.61	J/mol×K	792.49	Joback Method
cpg	550.13	J/mol×K	754.68	Joback Method
cpg	534.50	J/mol×K	716.88	Joback Method
cpg	517.66	J/mol×K	679.07	Joback Method
cpg	590.37	J/mol×K	868.11	Joback Method
dvisc	0.0001198	Pa×s	641.26	Joback Method
dvisc	0.0001555	Pa×s	591.91	Joback Method

dvisc	0.0002116	Pa×s	542.56	Joback Method
dvisc	0.0003063	Pa×s	493.21	Joback Method
dvisc	0.0004815	Pa×s	443.85	Joback Method
dvisc	0.0008474	Pa×s	394.50	Joback Method
dvisc	0.0017532	Pa×s	345.15	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R255880&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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