

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(CCOCc2ccccc2)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
rinqol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0002116	Paxs	542.56	Joback Method
dvisc	0.0003063	Paxs	493.21	Joback Method
dvisc	0.0004815	Paxs	443.85	Joback Method
dvisc	0.0008474	Paxs	394.50	Joback Method
dvisc	0.0017532	Paxs	345.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R255880&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mccvol:	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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