Fumaric acid, 2-phenethyl cyclohexylmethyl ester

Inchi: InChI=1S/C19H24O4/c20-18(22-14-13-16-7-3-1-4-8-16)11-12-19(21)23-15-17-9-5-2-6-10

InchiKey: GZUJZOLYRPCMPI-VAWYXSNFSA-N

Formula: C19H24O4

SMILES: O=C(C=CC(=O)OCC1CCCCC1)OCCc1ccccc1

Mol. weight [g/mol]: 316.39

Physical Properties

Property code	Value	Unit	Source
gf	-141.66	kJ/mol	Joback Method
hf	-517.02	kJ/mol	Joback Method
hfus	36.62	kJ/mol	Joback Method
hvap	78.86	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.452		Crippen Method
mcvol	254.530	ml/mol	McGowan Method
pc	1792.42	kPa	Joback Method
rinpol	2477.00		NIST Webbook
rinpol	2477.00		NIST Webbook
tb	837.09	K	Joback Method
tc	1063.77	K	Joback Method
tf	476.93	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.38	J/mol×K	837.09	Joback Method
cpg	805.10	J/mol×K	874.87	Joback Method
cpg	820.39	J/mol×K	912.65	Joback Method
cpg	834.30	J/mol×K	950.43	Joback Method
cpg	846.89	J/mol×K	988.21	Joback Method
cpg	858.22	J/mol×K	1025.99	Joback Method
cpg	868.34	J/mol×K	1063.77	Joback Method
dvisc	0.0008187	Pa×s	476.93	Joback Method

dvisc	0.0004081	Pa×s	536.96	Joback Method
dvisc	0.0002340	Pa×s	596.98	Joback Method
dvisc	0.0001486	Pa×s	657.01	Joback Method
dvisc	0.0001017	Pa×s	717.04	Joback Method
dvisc	0.0000739	Pa×s	777.06	Joback Method
dvisc	0.0000562	Pa×s	837.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405682&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