Fumaric acid, monoamide, N-methyl-N-phenyl-, neopentyl ester

Inchi: InChI=1S/C16H21NO3/c1-16(2,3)12-20-15(19)11-10-14(18)17(4)13-8-6-5-7-9-13/h5-11H

InchiKey: WMLZHRQDEIMTGP-ZHACJKMWSA-N

Formula: C16H21NO3

SMILES: CN(C(=O)C=CC(=O)OCC(C)(C)C)c1ccccc1

Mol. weight [g/mol]: 275.34

Physical Properties

Property code	Value	Unit	Source
gf	27.25	kJ/mol	Joback Method
hf	-318.42	kJ/mol	Joback Method
hfus	31.43	kJ/mol	Joback Method
hvap	70.09	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.795		Crippen Method
mcvol	227.230	ml/mol	McGowan Method
pc	1984.12	kPa	Joback Method
rinpol	2132.00		NIST Webbook
tb	735.69	K	Joback Method
tc	951.94	K	Joback Method
tf	448.40	K	Joback Method
vc	0.841	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	639.91	J/mol×K	735.69	Joback Method
cpg	655.51	J/mol×K	771.73	Joback Method
cpg	669.99	J/mol×K	807.77	Joback Method
cpg	683.43	J/mol×K	843.82	Joback Method
cpg	695.92	J/mol×K	879.86	Joback Method
cpg	707.54	J/mol×K	915.90	Joback Method
cpg	718.37	J/mol×K	951.94	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357512&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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