Fumaric acid, 2-phenethyl naphth-2-ylmethyl ester

Inchi: InChI=1S/C23H20O4/c24-22(26-15-14-18-6-2-1-3-7-18)12-13-23(25)27-17-19-10-11-20-

InchiKey: HGKOZGMNGATSAG-OUKQBFOZSA-N

Formula: C23H20O4

SMILES: O=C(C=CC(=O)OCc1ccc2ccccc2c1)OCCc1ccccc1

Mol. weight [g/mol]: 360.40

Physical Properties

Property code	Value	Unit	Source
gf	77.00	kJ/mol	Joback Method
hf	-237.77	kJ/mol	Joback Method
hfus	45.81	kJ/mol	Joback Method
hvap	91.92	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	4.225		Crippen Method
mcvol	278.530	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
rinpol	3080.00		NIST Webbook
rinpol	3080.00		NIST Webbook
tb	959.70	K	Joback Method
tc	1201.68	K	Joback Method
tf	586.27	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.64	J/mol×K	959.70	Joback Method
cpg	859.51	J/mol×K	1000.03	Joback Method
cpg	871.35	J/mol×K	1040.36	Joback Method
cpg	882.28	J/mol×K	1080.69	Joback Method
cpg	892.41	J/mol×K	1121.02	Joback Method
cpg	901.86	J/mol×K	1161.35	Joback Method
cpg	910.73	J/mol×K	1201.68	Joback Method
dvisc	0.0004595	Pa×s	586.27	Joback Method

dvisc	0.0002855	Pa×s	648.51	Joback Method
dvisc	0.0001928	Pa×s	710.75	Joback Method
dvisc	0.0001387	Pa×s	772.99	Joback Method
dvisc	0.0001048	Pa×s	835.22	Joback Method
dvisc	0.0000823	Pa×s	897.46	Joback Method
dvisc	0.0000667	Pa×s	959.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405686&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