Fumaric acid, hexyl 4-phenoxybenzyl ester

Inchi: InChI=1S/C23H26O5/c1-2-3-4-8-17-26-22(24)15-16-23(25)27-18-19-11-13-21(14-12-19)28-20-9-6-5-7-10-20/h5-7,9-16H,2-4,8,17-18H2,1H3/b16-15+

InchiKey: DJCCIZGIRQSSHP-FOCLMDBBSA-N

Formula: C23H26O5

SMILES: CCCCCCOC(=O)C=CC(=O)OCc1ccc(Oc2ccccc2)cc1

Mol. weight [g/mol]: 382.45

Physical Properties

Property code	Value	Unit	Source
gf	-134.65	kJ/mol	Joback Method
hf	-561.06	kJ/mol	Joback Method
hfus	49.98	kJ/mol	Joback Method
hvap	92.69	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	5.202		Crippen Method
mcvol	303.860	ml/mol	McGowan Method
pc	1421.85	kPa	Joback Method
rinpol	2910.00		NIST Webbook
rinpol	2910.00		NIST Webbook
tb	963.14	K	Joback Method
tc	1189.95	K	Joback Method
tf	575.80	K	Joback Method
vc	1.153	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	955.81	J/mol×K	963.14	Joback Method
cpg	1009.16	J/mol×K	1152.15	Joback Method
cpg	1001.01	J/mol×K	1114.35	Joback Method
cpg	991.65	J/mol×K	1076.55	Joback Method
cpg	981.03	J/mol×K	1038.74	Joback Method
cpg	969.10	J/mol×K	1000.94	Joback Method
cpg	1016.15	J/mol×K	1189.95	Joback Method
dvisc	0.0000240	Pa×s	963.14	Joback Method

dvisc	0.0000307	Pa×s	898.58	Joback Method
dvisc	0.0000409	Pa×s	834.03	Joback Method
dvisc	0.0000572	Pa×s	769.47	Joback Method
dvisc	0.0000850	Pa×s	704.91	Joback Method
dvisc	0.0001367	Pa×s	640.36	Joback Method
dvisc	0.0002448	Pa×s	575.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348115&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