Fumaric acid, isohexyl 4-phenoxybenzyl ester

Inchi: InChI=1S/C23H26O5/c1-18(2)7-6-16-26-22(24)14-15-23(25)27-17-19-10-12-21(13-11-19
InchiKey: GNFCZMQYLXYVTP-CCEZHUSRSA-N
Formula: C23H26O5
SMILES: CC(C)CCCOC(=O)C=CC(=O)OCc1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]: 382.45

Physical Properties

Property code	Value	Unit	Source
gf	-137.09	kJ/mol	Joback Method
hf	-566.34	kJ/mol	Joback Method
hfus	46.46	kJ/mol	Joback Method
hvap	92.30	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	5.058		Crippen Method
mcvol	303.860	ml/mol	McGowan Method
pc	1430.46	kPa	Joback Method
rinpol	2867.00		NIST Webbook
rinpol	2867.00		NIST Webbook
tb	962.70	K	Joback Method
tc	1191.34	K	Joback Method
tf	560.80	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	956.26	J/mol×K	962.70	Joback Method
cpg	969.59	J/mol×K	1000.81	Joback Method
cpg	981.53	J/mol×K	1038.91	Joback Method
cpg	992.13	J/mol×K	1077.02	Joback Method
cpg	1001.43	J/mol×K	1115.13	Joback Method
cpg	1009.50	J/mol×K	1153.23	Joback Method
cpg	1016.37	J/mol×K	1191.34	Joback Method
dvisc	0.0002673	Pa×s	560.80	Joback Method

dvisc	0.0001409	Pa×s	627.78	Joback Method
dvisc	0.0000841	Pa×s	694.77	Joback Method
dvisc	0.0000549	Pa×s	761.75	Joback Method
dvisc	0.0000384	Pa×s	828.73	Joback Method
dvisc	0.0000284	Pa×s	895.72	Joback Method
dvisc	0.0000218	Pa×s	962.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348114&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