Fumaric acid, heptyl 4-phenoxybenzyl ester

Inchi: InChI=1S/C24H28O5/c1-2-3-4-5-9-18-27-23(25)16-17-24(26)28-19-20-12-14-22(15-13-2
InchiKey: DBHCSXJYMMWFKK-WUKNDPDISA-N
Formula: C24H28O5
SMILES: CCCCCCCOC(=O)C=CC(=O)OCc1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]: 396.48

Physical Properties

Property code	Value	Unit	Source
gf	-126.23	kJ/mol	Joback Method
hf	-581.70	kJ/mol	Joback Method
hfus	52.57	kJ/mol	Joback Method
hvap	94.91	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.592		Crippen Method
mcvol	317.950	ml/mol	McGowan Method
pc	1324.24	kPa	Joback Method
rinpol	3012.00		NIST Webbook
tb	986.02	K	Joback Method
tc	1213.88	K	Joback Method
tf	587.07	K	Joback Method
vc	1.210	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1015.30	J/mol×K	986.02	Joback Method
cpg	1068.61	J/mol×K	1175.90	Joback Method
cpg	1060.52	J/mol×K	1137.92	Joback Method
cpg	1051.19	J/mol×K	1099.95	Joback Method
cpg	1040.58	J/mol×K	1061.97	Joback Method
cpg	1028.64	J/mol×K	1024.00	Joback Method
cpg	1075.54	J/mol×K	1213.88	Joback Method
dvisc	0.0000207	Pa×s	986.02	Joback Method
dvisc	0.0000266	Pa×s	919.53	Joback Method

dvisc	0.0000355	Pa×s	853.04	Joback Method
dvisc	0.0000499	Pa×s	786.54	Joback Method
dvisc	0.0000745	Pa×s	720.05	Joback Method
dvisc	0.0001208	Pa×s	653.56	Joback Method
dvisc	0.0002185	Pa×s	587.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348116&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

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