Fumaric acid, dodecyl 4-phenoxybenzyl ester

Inchi: InChI=1S/C29H38O5/c1-2-3-4-5-6-7-8-9-10-14-23-32-28(30)21-22-29(31)33-24-25-17-19
InchiKey: KKDQGLCUBLUSHV-QURGRASLSA-N
Formula: C29H38O5
SMILES: CCCCCCCCCCCCOC(=O)C=CC(=O)OCc1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]: 466.61

Physical Properties

Property code	Value	Unit	Source
gf	-84.13	kJ/mol	Joback Method
hf	-684.90	kJ/mol	Joback Method
hfus	65.52	kJ/mol	Joback Method
hvap	106.04	kJ/mol	Joback Method
log10ws	-8.26		Crippen Method
logp	7.542		Crippen Method
mcvol	388.400	ml/mol	McGowan Method
pc	959.69	kPa	Joback Method
rinpol	3694.00		NIST Webbook
rinpol	3694.00		NIST Webbook
tb	1100.42	K	Joback Method
tc	1348.45	K	Joback Method
tf	643.42	K	Joback Method
vc	1.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1319.38	J/mol×K	1100.42	Joback Method
cpg	1372.39	J/mol×K	1307.11	Joback Method
cpg	1364.77	J/mol×K	1265.78	Joback Method
cpg	1355.75	J/mol×K	1224.44	Joback Method
cpg	1345.25	J/mol×K	1183.10	Joback Method
cpg	1333.16	J/mol×K	1141.76	Joback Method
cpg	1378.70	J/mol×K	1348.45	Joback Method
dvisc	0.0000096	Pa×s	1100.42	Joback Method

dvisc	0.0000125	Pa×s	1024.25	Joback Method
dvisc	0.0000170	Pa×s	948.09	Joback Method
dvisc	0.0000243	Pa×s	871.92	Joback Method
dvisc	0.0000373	Pa×s	795.75	Joback Method
dvisc	0.0000626	Pa×s	719.59	Joback Method
dvisc	0.0001187	Pa×s	643.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348122&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