Fumaric acid, 2-methoxyphenyl cyclohexylmethyl ester

Inchi: InChI=1S/C18H22O5/c1-21-15-9-5-6-10-16(15)23-18(20)12-11-17(19)22-13-14-7-3-2-4-8

InchiKey: UZFWSYVAHCBDFQ-VAWYXSNFSA-N

Formula: C18H22O5

SMILES: COc1ccccc1OC(=O)C=CC(=O)OCC1CCCCC1

Mol. weight [g/mol]: 318.36

Physical Properties

Property code	Value	Unit	Source
gf	-264.71	kJ/mol	Joback Method
hf	-640.07	kJ/mol	Joback Method
hfus	34.83	kJ/mol	Joback Method
hvap	79.71	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.280		Crippen Method
mcvol	246.310	ml/mol	McGowan Method
pc	1893.65	kPa	Joback Method
rinpol	2475.00		NIST Webbook
rinpol	2475.00		NIST Webbook
tb	841.61	K	Joback Method
tc	1069.89	K	Joback Method
tf	500.41	K	Joback Method
vc	0.914	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	758.00	J/mol×K	841.61	Joback Method
cpg	773.85	J/mol×K	879.66	Joback Method
cpg	788.23	J/mol×K	917.70	Joback Method
cpg	801.17	J/mol×K	955.75	Joback Method
cpg	812.69	J/mol×K	993.79	Joback Method
cpg	822.81	J/mol×K	1031.84	Joback Method
cpg	831.57	J/mol×K	1069.89	Joback Method
dvisc	0.0005349	Pa×s	500.41	Joback Method

dvisc	0.0002933	Pa×s	557.28	Joback Method
dvisc	0.0001798	Pa×s	614.14	Joback Method
dvisc	0.0001197	Pa×s	671.01	Joback Method
dvisc	0.0000849	Pa×s	727.88	Joback Method
dvisc	0.0000633	Pa×s	784.74	Joback Method
dvisc	0.0000492	Pa×s	841.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405935&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