Fumaric acid, 3-phenylpropyl cyclohexylmethyl ester

Inchi: InChI=1S/C20H26O4/c21-19(23-15-7-12-17-8-3-1-4-9-17)13-14-20(22)24-16-18-10-5-2-6-11-18/h1,3-4,8-9,13-14,18H,2,5-7,10-12,15-16H2/b14-13+

InchiKey: XUCLDZYJGXOFLW-BUHFOSPRSA-N

Formula: C20H26O4

SMILES: O=C(C=CC(=O)OCC1CCCCC1)OCCCc1ccccc1

Mol. weight [g/mol]: 330.42

Physical Properties

Property code	Value	Unit	Source
gf	-133.24	kJ/mol	Joback Method
hf	-537.66	kJ/mol	Joback Method
hfus	39.21	kJ/mol	Joback Method
hvap	81.09	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	3.842		Crippen Method
mcvol	268.620	ml/mol	McGowan Method
pc	1655.15	kPa	Joback Method
rinpol	2606.00		NIST Webbook
tb	859.97	K	Joback Method
tc	1084.33	K	Joback Method
tf	488.20	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.80	J/mol×K	859.97	Joback Method
cpg	863.50	J/mol×K	897.36	Joback Method
cpg	878.77	J/mol×K	934.76	Joback Method
cpg	892.67	J/mol×K	972.15	Joback Method
cpg	905.24	J/mol×K	1009.54	Joback Method
cpg	916.56	J/mol×K	1046.94	Joback Method
cpg	926.67	J/mol×K	1084.33	Joback Method
dvisc	0.0007360	Pa×s	488.20	Joback Method
dvisc	0.0003630	Pa×s	550.16	Joback Method

dvisc	0.0002066	Pa×s	612.12	Joback Method
dvisc	0.0001304	Pa×s	674.09	Joback Method
dvisc	0.0000889	Pa×s	736.05	Joback Method
dvisc	0.0000644	Pa×s	798.01	Joback Method
dvisc	0.0000488	Pa×s	859.97	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405668&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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