

Glutaric acid, 4-methoxyphenyl propyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C15H20O5/c1-3-11-19-14(16)5-4-6-15(17)20-13-9-7-12(18-2)8-10-13/h7-10H,3

IGSKIKKCDIVVOX-UHFFFAOYSA-N

C15H20O5

CCCOC(=O)CCCC(=O)Oc1ccc(OC)cc1

280.32

Physical Properties

Property code	Value	Unit	Source
gf	-394.64	kJ/mol	Joback Method
hf	-749.69	kJ/mol	Joback Method
hfus	35.02	kJ/mol	Joback Method
hvap	72.64	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.724		Crippen Method
mcvol	219.200	ml/mol	McGowan Method
pc	1945.79	kPa	Joback Method
rinpol	2176.00		NIST Webbook
rinpol	2176.00		NIST Webbook
tb	749.26	K	Joback Method
tc	951.78	K	Joback Method
tf	464.30	K	Joback Method
vc	0.834	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.91	J/mol×K	749.26	Joback Method
cpg	635.35	J/mol×K	783.01	Joback Method
cpg	648.83	J/mol×K	816.77	Joback Method
cpg	661.35	J/mol×K	850.52	Joback Method
cpg	672.91	J/mol×K	884.27	Joback Method
cpg	683.50	J/mol×K	918.02	Joback Method
cpg	693.12	J/mol×K	951.78	Joback Method
dvisc	0.0006625	Pa×s	464.30	Joback Method

dvisc	0.0003969	Pa×s	511.79	Joback Method
dvisc	0.0002594	Pa×s	559.29	Joback Method
dvisc	0.0001812	Pa×s	606.78	Joback Method
dvisc	0.0001333	Pa×s	654.27	Joback Method
dvisc	0.0001023	Pa×s	701.77	Joback Method
dvisc	0.0000811	Pa×s	749.26	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
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=U358737&Units=SI

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log_{10ws}:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
rin_{pol}:	Non-polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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