

Glutaric acid, di(2-methoxybenzyl) ester

Inchi:	InChI=1S/C21H24O6/c1-24-18-10-5-3-8-16(18)14-26-20(22)12-7-13-21(23)27-15-17-9-4
InchiKey:	CAWYSROFZZLTBW-UHFFFAOYSA-N
Formula:	C21H24O6
SMILES:	COc1ccccc1COC(=O)CCCC(=O)OCc1ccccc1OC
Mol. weight [g/mol]:	372.41

Physical Properties

Property code	Value	Unit	Source
gf	-346.34	kJ/mol	Joback Method
hf	-780.69	kJ/mol	Joback Method
hfus	45.40	kJ/mol	Joback Method
hvap	91.35	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	3.661		Crippen Method
mvol	285.850	ml/mol	McGowan Method
pc	1545.13	kPa	Joback Method
rinpol	2952.00		NIST Webbook
tb	940.62	K	Joback Method
tc	1164.12	K	Joback Method
tf	593.09	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	892.45	J/molxK	940.62	Joback Method
cpg	939.47	J/molxK	1126.87	Joback Method
cpg	933.16	J/molxK	1089.62	Joback Method
cpg	925.31	J/molxK	1052.37	Joback Method
cpg	915.90	J/molxK	1015.12	Joback Method
cpg	904.95	J/molxK	977.87	Joback Method
cpg	944.24	J/molxK	1164.12	Joback Method
dvisc	0.0000278	Paxs	940.62	Joback Method
dvisc	0.0000348	Paxs	882.70	Joback Method

dvisc	0.0000451	Paxs	824.78	Joback Method
dvisc	0.0000606	Paxs	766.86	Joback Method
dvisc	0.0000855	Paxs	708.93	Joback Method
dvisc	0.0001283	Paxs	651.01	Joback Method
dvisc	0.0002084	Paxs	593.09	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376941&Units=SI

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

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