

Glutaric acid, isobutyl 3-phenoxybenzyl ester

Inchi:	InChI=1S/C22H26O5/c1-17(2)15-25-21(23)12-7-13-22(24)26-16-18-8-6-11-20(14-18)27-
InchiKey:	DTGOAXVCWRTXFL-UHFFFAOYSA-N
Formula:	C22H26O5
SMILES:	CC(C)COC(=O)CCCC(=O)OCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]:	370.44

Physical Properties

Property code	Value	Unit	Source
gf	-225.73	kJ/mol	Joback Method
hf	-662.92	kJ/mol	Joback Method
hfus	43.67	kJ/mol	Joback Method
hvap	90.11	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.892		Crippen Method
mcvol	294.070	ml/mol	McGowan Method
pc	1479.29	kPa	Joback Method
rinpola	2807.00		NIST Webbook
tb	935.66	K	Joback Method
tc	1159.79	K	Joback Method
tf	554.61	K	Joback Method
vc	1.111	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	925.83	J/molxK	935.66	Joback Method
cpg	979.34	J/molxK	1122.44	Joback Method
cpg	971.47	J/molxK	1085.08	Joback Method
cpg	962.21	J/molxK	1047.73	Joback Method
cpg	951.53	J/molxK	1010.37	Joback Method
cpg	939.42	J/molxK	973.02	Joback Method
cpg	985.86	J/molxK	1159.79	Joback Method
dvisc	0.0000289	Paxs	935.66	Joback Method
dvisc	0.0000373	Paxs	872.15	Joback Method

dvisc	0.0000502	Paxs	808.64	Joback Method
dvisc	0.0000710	Paxs	745.13	Joback Method
dvisc	0.0001072	Paxs	681.63	Joback Method
dvisc	0.0001761	Paxs	618.12	Joback Method
dvisc	0.0003243	Paxs	554.61	Joback Method

Sources

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=U359255&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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