Glutaric acid, butyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C22H26O5/c1-2-3-15-25-21(23)13-8-14-22(24)26-17-18-9-7-12-20(16-18)27-1
InchiKey: RYWXBSFWRKPRBH-UHFFFAOYSA-N
Formula: C22H26O5
SMILES: CCCCOC(=O)CCCC(=O)OCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]: 370.44

Physical Properties

Property code	Value	Unit	Source
gf	-223.29	kJ/mol	Joback Method
hf	-657.64	kJ/mol	Joback Method
hfus	47.19	kJ/mol	Joback Method
hvap	90.50	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	5.036		Crippen Method
mcvol	294.070	ml/mol	McGowan Method
pc	1470.23	kPa	Joback Method
rinpol	2856.00		NIST Webbook
rinpol	2856.00		NIST Webbook
tb	936.10	K	Joback Method
tc	1158.31	K	Joback Method
tf	569.61	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	925.35	J/mol×K	936.10	Joback Method
cpg	938.87	J/mol×K	973.14	Joback Method
cpg	950.95	J/mol×K	1010.17	Joback Method
cpg	961.63	J/mol×K	1047.21	Joback Method
cpg	970.94	J/mol×K	1084.24	Joback Method
cpg	978.89	J/mol×K	1121.28	Joback Method
cpg	985.53	J/mol×K	1158.31	Joback Method
dvisc	0.0002967	Pa×s	569.61	Joback Method

dvisc	0.0001706	Pa×s	630.69	Joback Method
dvisc	0.0001081	Pa×s	691.77	Joback Method
dvisc	0.0000738	Pa×s	752.86	Joback Method
dvisc	0.0000533	Pa×s	813.94	Joback Method
dvisc	0.0000403	Pa×s	875.02	Joback Method
dvisc	0.0000316	Pa×s	936.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359256&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

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