

Glutaric acid, butyl 5-methoxy-3-phenylpentyl ester

Inchi:	InChI=1S/C21H32O5/c1-3-4-15-25-20(22)11-8-12-21(23)26-17-14-19(13-16-24-2)18-9-6
InchiKey:	TWKGJBJUEOCOFQ-UHFFFAOYSA-N
Formula:	C21H32O5
SMILES:	CCCCOC(=O)CCCC(=O)OCCC(CCOC)c1ccccc1
Mol. weight [g/mol]:	364.48

Physical Properties

Property code	Value	Unit	Source
gf	-336.93	kJ/mol	Joback Method
hf	-867.34	kJ/mol	Joback Method
hfus	47.43	kJ/mol	Joback Method
hvap	84.95	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	4.254		Crippen Method
mcvol	303.740	ml/mol	McGowan Method
pc	1257.48	kPa	Joback Method
rinpola	2608.00		NIST Webbook
tb	881.12	K	Joback Method
tc	1084.74	K	Joback Method
tf	504.40	K	Joback Method
vc	1.163	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	967.89	J/molxK	881.12	Joback Method
cpg	983.88	J/molxK	915.06	Joback Method
cpg	998.58	J/molxK	948.99	Joback Method
cpg	1012.01	J/molxK	982.93	Joback Method
cpg	1024.19	J/molxK	1016.86	Joback Method
cpg	1035.13	J/molxK	1050.80	Joback Method
cpg	1044.86	J/molxK	1084.74	Joback Method
dvisc	0.0004899	Paxs	504.40	Joback Method
dvisc	0.0002418	Paxs	567.19	Joback Method

dvisc	0.0001374	Paxs	629.97	Joback Method
dvisc	0.0000865	Paxs	692.76	Joback Method
dvisc	0.0000588	Paxs	755.55	Joback Method
dvisc	0.0000424	Paxs	818.33	Joback Method
dvisc	0.0000320	Paxs	881.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359530&Units=SI
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

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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