Glutaric acid, isobutyl 3-phenylpropyl ester

Inchi: InChI=1S/C18H26O4/c1-15(2)14-22-18(20)12-6-11-17(19)21-13-7-10-16-8-4-3-5-9-16/h3
InchiKey: BFCYNWPDZPQZKK-UHFFFAOYSA-N
Formula: C18H26O4
SMILES: CC(C)COC(=O)CCCC(=O)OCCCc1ccccc1
Mol. weight [g/mol]: 306.40

Physical Properties

Property code	Value	Unit	Source
gf	-257.19	kJ/mol	Joback Method
hf	-673.20	kJ/mol	Joback Method
hfus	38.47	kJ/mol	Joback Method
hvap	75.86	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.532		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1580.97	kPa	Joback Method
rinpol	2291.00		NIST Webbook
rinpol	2291.00		NIST Webbook
tb	790.06	K	Joback Method
tc	991.28	K	Joback Method
tf	448.36	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.47	J/mol×K	790.06	Joback Method
cpg	831.62	J/mol×K	957.74	Joback Method
cpg	819.87	J/mol×K	924.21	Joback Method
cpg	807.11	J/mol×K	890.67	Joback Method
cpg	793.30	J/mol×K	857.13	Joback Method
cpg	778.43	J/mol×K	823.60	Joback Method
cpg	842.38	J/mol×K	991.28	Joback Method
dvisc	0.0000657	Pa×s	790.06	Joback Method

dvisc	0.0000866	Pa×s	733.11	Joback Method
dvisc	0.0001197	Pa×s	676.16	Joback Method
dvisc	0.0001755	Pa×s	619.21	Joback Method
dvisc	0.0002780	Pa×s	562.26	Joback Method
dvisc	0.0004886	Pa×s	505.31	Joback Method
dvisc	0.0009909	Pa×s	448.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360131&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