

Glutaric acid, isobutyl 1-phenylpropyl ester

Inchi:	InChI=1S/C18H26O4/c1-4-16(15-9-6-5-7-10-15)22-18(20)12-8-11-17(19)21-13-14(2)3/h5
InchiKey:	WCHRCTSVLIGPMM-UHFFFAOYSA-N
Formula:	C18H26O4
SMILES:	CCC(OC(=O)CCCC(=O)OCC(C)C)c1ccccc1
Mol. weight [g/mol]:	306.40

Physical Properties

Property code	Value	Unit	Source
gf	-259.63	kJ/mol	Joback Method
hf	-678.48	kJ/mol	Joback Method
hfus	34.94	kJ/mol	Joback Method
hvap	75.47	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	4.050		Crippen Method
mvol	255.600	ml/mol	McGowan Method
pc	1591.08	kPa	Joback Method
rinpol	2129.00		NIST Webbook
rinpol	2129.00		NIST Webbook
tb	789.62	K	Joback Method
tc	993.35	K	Joback Method
tf	433.36	K	Joback Method
vc	0.972	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	763.01	J/molxK	789.62	Joback Method
cpg	779.16	J/molxK	823.58	Joback Method
cpg	794.20	J/molxK	857.53	Joback Method
cpg	808.13	J/molxK	891.49	Joback Method
cpg	820.99	J/molxK	925.44	Joback Method
cpg	832.79	J/molxK	959.40	Joback Method
cpg	843.56	J/molxK	993.35	Joback Method
dvisc	0.0011751	Paxs	433.36	Joback Method

dvisc	0.0005318	Paxs	492.74	Joback Method
dvisc	0.0002855	Paxs	552.11	Joback Method
dvisc	0.0001729	Paxs	611.49	Joback Method
dvisc	0.0001144	Paxs	670.87	Joback Method
dvisc	0.0000810	Paxs	730.24	Joback Method
dvisc	0.0000604	Paxs	789.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358949&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

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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