

Glutaric acid, hexyl 3-methylbenzyl ester

Inchi:	InChI=1S/C19H28O4/c1-3-4-5-6-13-22-18(20)11-8-12-19(21)23-15-17-10-7-9-16(2)14-17
InchiKey:	XBJKVWCXRBBFAG-UHFFFAOYSA-N
Formula:	C19H28O4
SMILES:	CCCCCOC(=O)CCCC(=O)OCc1cccc(C)c1
Mol. weight [g/mol]:	320.42

Physical Properties

Property code	Value	Unit	Source
gf	-255.96	kJ/mol	Joback Method
hf	-700.03	kJ/mol	Joback Method
hfus	44.19	kJ/mol	Joback Method
hvap	79.14	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.332		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1441.35	kPa	Joback Method
rinpola	2621.00		NIST Webbook
tb	818.36	K	Joback Method
tc	1017.87	K	Joback Method
tf	487.15	K	Joback Method
vc	1.040	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.06	J/molxK	818.36	Joback Method
cpg	887.96	J/molxK	984.62	Joback Method
cpg	876.27	J/molxK	951.37	Joback Method
cpg	863.56	J/molxK	918.12	Joback Method
cpg	849.80	J/molxK	884.86	Joback Method
cpg	834.97	J/molxK	851.61	Joback Method
cpg	898.65	J/molxK	1017.87	Joback Method
dvisc	0.0000629	Paxs	818.36	Joback Method
dvisc	0.0000807	Paxs	763.16	Joback Method

dvisc	0.0001077	Paxs	707.96	Joback Method
dvisc	0.0001507	Paxs	652.75	Joback Method
dvisc	0.0002246	Paxs	597.55	Joback Method
dvisc	0.0003630	Paxs	542.35	Joback Method
dvisc	0.0006541	Paxs	487.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377651&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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