

Glutaric acid, hexyl 3-iodobenzyl ester

Inchi:	InChI=1S/C18H25IO4/c1-2-3-4-5-12-22-17(20)10-7-11-18(21)23-14-15-8-6-9-16(19)13-1
InchiKey:	HKPMCRLFKHSMMG-UHFFFAOYSA-N
Formula:	C18H25IO4
SMILES:	CCCCCOC(=O)CCCC(=O)OCc1cccc(I)c1
Mol. weight [g/mol]:	432.29

Physical Properties

Property code	Value	Unit	Source
gf	-206.26	kJ/mol	Joback Method
hf	-602.52	kJ/mol	Joback Method
hfus	46.01	kJ/mol	Joback Method
hvap	86.28	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	4.628		Crippen Method
mvol	281.420	ml/mol	McGowan Method
pc	1525.88	kPa	Joback Method
rinpol	2709.00		NIST Webbook
rinpol	2709.00		NIST Webbook
tb	888.62	K	Joback Method
tc	1107.61	K	Joback Method
tf	533.94	K	Joback Method
vc	1.071	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	812.55	J/molxK	888.62	Joback Method
cpg	869.73	J/molxK	1071.11	Joback Method
cpg	860.40	J/molxK	1034.61	Joback Method
cpg	850.05	J/molxK	998.12	Joback Method
cpg	838.65	J/molxK	961.62	Joback Method
cpg	826.16	J/molxK	925.12	Joback Method
cpg	878.08	J/molxK	1107.61	Joback Method
dvisc	0.0000524	Paxs	888.62	Joback Method

dvisc	0.0000670	Paxs	829.51	Joback Method
dvisc	0.0000891	Paxs	770.39	Joback Method
dvisc	0.0001242	Paxs	711.28	Joback Method
dvisc	0.0001839	Paxs	652.17	Joback Method
dvisc	0.0002945	Paxs	593.05	Joback Method
dvisc	0.0005232	Paxs	533.94	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376988&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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