

Glutaric acid, 3-iodobenzyl 2-methylhex-3-yl ester

Inchi:	InChI=1S/C19H27IO4/c1-4-7-17(14(2)3)24-19(22)11-6-10-18(21)23-13-15-8-5-9-16(20)1
InchiKey:	WHGZNIHEDPWURF-UHFFFAOYSA-N
Formula:	C19H27IO4
SMILES:	CCCC(OC(=O)CCCC(=O)OCc1cccc(I)c1)C(C)C
Mol. weight [g/mol]:	446.32

Physical Properties

Property code	Value	Unit	Source
gf	-202.72	kJ/mol	Joback Method
hf	-633.72	kJ/mol	Joback Method
hfus	41.55	kJ/mol	Joback Method
hvap	87.73	kJ/mol	Joback Method
log10ws	-6.12		Crippen Method
logp	4.873		Crippen Method
mcvol	295.510	ml/mol	McGowan Method
pc	1434.80	kPa	Joback Method
rinpol	2662.00		NIST Webbook
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tb	910.62	K	Joback Method
tc	1133.59	K	Joback Method
tf	515.21	K	Joback Method
vc	1.115	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.72	J/molxK	910.62	Joback Method
cpg	929.77	J/molxK	1096.43	Joback Method
cpg	920.45	J/molxK	1059.27	Joback Method
cpg	910.02	J/molxK	1022.11	Joback Method
cpg	898.45	J/molxK	984.94	Joback Method
cpg	885.69	J/molxK	947.78	Joback Method
cpg	938.03	J/molxK	1133.59	Joback Method
dvisc	0.0000376	Paxs	910.62	Joback Method

dvisc	0.0000496	Paxs	844.72	Joback Method
dvisc	0.0000687	Paxs	778.82	Joback Method
dvisc	0.0001010	Paxs	712.91	Joback Method
dvisc	0.0001607	Paxs	647.01	Joback Method
dvisc	0.0002840	Paxs	581.11	Joback Method
dvisc	0.0005807	Paxs	515.21	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=U376987&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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