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

Inchi: InChI=1S/C19H27IO4/c1-4-8-17(14(2)3)24-19(22)12-7-11-18(21)23-13-15-9-5-6-10-16(1

InchiKey: ZKCAIARMMXSMKU-UHFFFAOYSA-N

Formula: C19H27IO4

SMILES: CCCC(OC(=O)CCCC(=O)OCc1ccccc1I)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	2632.00		NIST Webbook
rinpol	2632.00		NIST Webbook
tb	910.62	K	Joback Method
tc	1133.59	K	Joback Method
tf	515.21	K	Joback Method
vc	1.115	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.72	J/mol×K	910.62	Joback Method
cpg	885.69	J/mol×K	947.78	Joback Method
cpg	898.45	J/mol×K	984.94	Joback Method
cpg	910.02	J/mol×K	1022.11	Joback Method
cpg	920.45	J/mol×K	1059.27	Joback Method
cpg	929.77	J/mol×K	1096.43	Joback Method
cpg	938.03	J/mol×K	1133.59	Joback Method
dvisc	0.0005807	Pa×s	515.21	Joback Method

dvisc	0.0002840	Pa×s	581.11	Joback Method
dvisc	0.0001607	Pa×s	647.01	Joback Method
dvisc	0.0001010	Pa×s	712.91	Joback Method
dvisc	0.0000687	Pa×s	778.82	Joback Method
dvisc	0.0000496	Pa×s	844.72	Joback Method
dvisc	0.0000376	Pa×s	910.62	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=U376880&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