

Glutaric acid, butyl 3-iodobenzyl ester

Inchi: InChI=1S/C16H21IO4/c1-2-3-10-20-15(18)8-5-9-16(19)21-12-13-6-4-7-14(17)11-13/h4,6
InchiKey: WCXPCLKJNIKXEB-UHFFFAOYSA-N
Formula: C16H21IO4
SMILES: CCCCO(=O)CCCC(=O)OCc1cccc(I)c1
Mol. weight [g/mol]: 404.24

Physical Properties

Property code	Value	Unit	Source
gf	-223.10	kJ/mol	Joback Method
hf	-561.24	kJ/mol	Joback Method
hfus	40.83	kJ/mol	Joback Method
hvap	81.83	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	3.848		Crippen Method
mvol	253.240	ml/mol	McGowan Method
pc	1783.35	kPa	Joback Method
rinpol	2500.00		NIST Webbook
rinpol	2500.00		NIST Webbook
tb	842.86	K	Joback Method
tc	1064.56	K	Joback Method
tf	511.40	K	Joback Method
vc	0.960	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	698.57	J/molxK	842.86	Joback Method
cpg	711.76	J/molxK	879.81	Joback Method
cpg	723.88	J/molxK	916.76	Joback Method
cpg	734.96	J/molxK	953.71	Joback Method
cpg	745.04	J/molxK	990.66	Joback Method
cpg	754.13	J/molxK	1027.61	Joback Method
cpg	762.27	J/molxK	1064.56	Joback Method
dvisc	0.0006500	Paxs	511.40	Joback Method

dvisc	0.0003746	Paxs	566.64	Joback Method
dvisc	0.0002381	Paxs	621.89	Joback Method
dvisc	0.0001629	Paxs	677.13	Joback Method
dvisc	0.0001181	Paxs	732.37	Joback Method
dvisc	0.0000895	Paxs	787.62	Joback Method
dvisc	0.0000704	Paxs	842.86	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=U376985&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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