Glutaric acid, butyl 2-iodobenzyl ester

Inchi: InChI=1S/C16H21IO4/c1-2-3-11-20-15(18)9-6-10-16(19)21-12-13-7-4-5-8-14(13)17/h4-5
InchiKey: TUHKBOZMEUAYBZ-UHFFFAOYSA-N
Formula: C16H21IO4
SMILES: CCCCOC(=O)CCCC(=O)OCc1ccccc1I
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
mcvol	253.240	ml/mol	McGowan Method
pc	1783.35	kPa	Joback Method
rinpol	2468.00		NIST Webbook
rinpol	2468.00		NIST Webbook
tb	842.86	K	Joback Method
tc	1064.56	K	Joback Method
tf	511.40	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	698.57	J/mol×K	842.86	Joback Method
cpg	754.13	J/mol×K	1027.61	Joback Method
cpg	745.04	J/mol×K	990.66	Joback Method
cpg	734.96	J/mol×K	953.71	Joback Method
cpg	723.88	J/mol×K	916.76	Joback Method
cpg	711.76	J/mol×K	879.81	Joback Method
cpg	762.27	J/mol×K	1064.56	Joback Method
dvisc	0.0000704	Pa×s	842.86	Joback Method

dvisc	0.0000895	Pa×s	787.62	Joback Method
dvisc	0.0001181	Pa×s	732.37	Joback Method
dvisc	0.0001629	Pa×s	677.13	Joback Method
dvisc	0.0002381	Pa×s	621.89	Joback Method
dvisc	0.0003746	Pa×s	566.64	Joback Method
dvisc	0.0006500	Pa×s	511.40	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U376878&Units=SI

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