

Glutaric acid, isohexyl tetrahydrofurfuryl ester

Inchi: InChI=1S/C16H28O5/c1-13(2)6-4-11-20-15(17)8-3-9-16(18)21-12-14-7-5-10-19-14/h13-1
InchiKey: FHIUYEAYXMPKGS-UHFFFAOYSA-N
Formula: C16H28O5
SMILES: CC(C)CCCOC(=O)CCCC(=O)OCC1CCCO1
Mol. weight [g/mol]: 300.39

Physical Properties

Property code	Value	Unit	Source
gf	-436.01	kJ/mol	Joback Method
hf	-939.97	kJ/mol	Joback Method
hfus	41.16	kJ/mol	Joback Method
hvap	73.90	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	2.858		Crippen Method
mcvol	246.190	ml/mol	McGowan Method
pc	1621.98	kPa	Joback Method
rinpol	2177.00		NIST Webbook
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tb	759.85	K	Joback Method
tc	954.50	K	Joback Method
tf	436.87	K	Joback Method
vc	0.935	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	760.27	J/molxK	759.85	Joback Method
cpg	777.51	J/molxK	792.29	Joback Method
cpg	793.67	J/molxK	824.73	Joback Method
cpg	808.78	J/molxK	857.18	Joback Method
cpg	822.85	J/molxK	889.62	Joback Method
cpg	835.90	J/molxK	922.06	Joback Method
cpg	847.95	J/molxK	954.50	Joback Method
dvisc	0.0015619	Paxs	436.87	Joback Method

dvisc	0.0007871	Paxs	490.70	Joback Method
dvisc	0.0004542	Paxs	544.53	Joback Method
dvisc	0.0002894	Paxs	598.36	Joback Method
dvisc	0.0001986	Paxs	652.19	Joback Method
dvisc	0.0001443	Paxs	706.02	Joback Method
dvisc	0.0001098	Paxs	759.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359661&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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