Glutaric acid, cyclohexylmethyl but-3-en-1-yl ester

Inchi: InChI=1S/C16H26O4/c1-2-3-12-19-15(17)10-7-11-16(18)20-13-14-8-5-4-6-9-14/h2,14H,1

InchiKey: HRLARGAGVLBNLS-UHFFFAOYSA-N

Formula: C16H26O4

SMILES: C=CCCOC(=O)CCCC(=O)OCC1CCCCC1

Mol. weight [g/mol]: 282.38

Physical Properties

Property code	Value	Unit	Source
gf	-271.71	kJ/mol	Joback Method
hf	-683.42	kJ/mol	Joback Method
hfus	33.32	kJ/mol	Joback Method
hvap	69.28	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.399		Crippen Method
mcvol	236.020	ml/mol	McGowan Method
pc	1714.61	kPa	Joback Method
rinpol	2025.00		NIST Webbook
rinpol	2025.00		NIST Webbook
tb	734.29	K	Joback Method
tc	933.21	K	Joback Method
tf	420.02	K	Joback Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	703.87	J/mol×K	734.29	Joback Method
cpg	721.72	J/mol×K	767.44	Joback Method
cpg	738.46	J/mol×K	800.60	Joback Method
cpg	754.08	J/mol×K	833.75	Joback Method
cpg	768.62	J/mol×K	866.90	Joback Method
cpg	782.09	J/mol×K	900.06	Joback Method
cpg	794.50	J/mol×K	933.21	Joback Method
dvisc	0.0014672	Pa×s	420.02	Joback Method

dvisc	0.0007361	Pa×s	472.40	Joback Method
dvisc	0.0004239	Pa×s	524.78	Joback Method
dvisc	0.0002698	Pa×s	577.15	Joback Method
dvisc	0.0001851	Pa×s	629.53	Joback Method
dvisc	0.0001346	Pa×s	681.91	Joback Method
dvisc	0.0001024	Pa×s	734.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U394039&Units=SI
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

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