Glutaric acid, (cyclohex-3-enyl)methyl 3-methylbut-2-yl ester

Inchi: InChI=1S/C17H28O4/c1-13(2)14(3)21-17(19)11-7-10-16(18)20-12-15-8-5-4-6-9-15/h4-5,

InchiKey: BADOUWWRKUBXRJ-UHFFFAOYSA-N

Formula: C17H28O4

SMILES: CC(C)C(C)OC(=O)CCCC(=O)OCC1CC=CCC1

Mol. weight [g/mol]: 296.40

Physical Properties

Property code	Value	Unit	Source
gf	-326.05	kJ/mol	Joback Method
hf	-782.27	kJ/mol	Joback Method
hfus	31.37	kJ/mol	Joback Method
hvap	71.69	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.644		Crippen Method
mcvol	250.110	ml/mol	McGowan Method
pc	1598.72	kPa	Joback Method
rinpol	2045.00		NIST Webbook
rinpol	2045.00		NIST Webbook
tb	758.77	K	Joback Method
tc	960.42	K	Joback Method
tf	403.81	K	Joback Method
vc	0.943	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.93	J/mol×K	758.77	Joback Method
cpg	780.10	J/mol×K	792.38	Joback Method
cpg	797.07	J/mol×K	825.99	Joback Method
cpg	812.85	J/mol×K	859.59	Joback Method
cpg	827.45	J/mol×K	893.20	Joback Method
cpg	840.90	J/mol×K	926.81	Joback Method
cpg	853.21	J/mol×K	960.42	Joback Method
dvisc	0.0018483	Pa×s	403.81	Joback Method

dvisc	0.0007737	Pa×s	462.97	Joback Method
dvisc	0.0003945	Pa×s	522.13	Joback Method
dvisc	0.0002307	Pa×s	581.29	Joback Method
dvisc	0.0001490	Pa×s	640.45	Joback Method
dvisc	0.0001036	Pa×s	699.61	Joback Method
dvisc	0.0000762	Pa×s	758.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405524&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