Glutaric acid, (cyclohex-3-enyl)methyl 3-methylbut-2-en-1-yl ester

Inchi: InChI=1S/C17H26O4/c1-14(2)11-12-20-16(18)9-6-10-17(19)21-13-15-7-4-3-5-8-15/h3-4,

InchiKey: WJMFVDLMUDJDBV-UHFFFAOYSA-N

Formula: C17H26O4

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

Mol. weight [g/mol]: 294.39

Physical Properties

Property code	Value	Unit	Source
gf	-249.50	kJ/mol	Joback Method
hf	-664.28	kJ/mol	Joback Method
hfus	37.31	kJ/mol	Joback Method
hvap	72.51	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.566		Crippen Method
mcvol	245.810	ml/mol	McGowan Method
pc	1652.46	kPa	Joback Method
rinpol	2154.00		NIST Webbook
tb	763.69	K	Joback Method
tc	968.02	K	Joback Method
tf	414.77	K	Joback Method
vc	0.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.20	J/mol×K	763.69	Joback Method
cpg	753.60	J/mol×K	797.75	Joback Method
cpg	769.85	J/mol×K	831.80	Joback Method
cpg	784.98	J/mol×K	865.86	Joback Method
cpg	799.03	J/mol×K	899.91	Joback Method
cpg	812.03	J/mol×K	933.97	Joback Method
cpg	824.00	J/mol×K	968.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405526&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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