

Glutaric acid, but-3-en-2-yl cyclohexylmethyl ester

Inchi:	InChI=1S/C16H26O4/c1-3-13(2)20-16(18)11-7-10-15(17)19-12-14-8-5-4-6-9-14/h3,13-14
InchiKey:	XKXGBIZFWUWDLR-UHFFFAOYSA-N
Formula:	C16H26O4
SMILES:	C=CC(C)OC(=O)CCCC(=O)OCC1CCCCC1
Mol. weight [g/mol]:	282.38

Physical Properties

Property code	Value	Unit	Source
gf	-274.15	kJ/mol	Joback Method
hf	-688.70	kJ/mol	Joback Method
hfus	29.80	kJ/mol	Joback Method
hvap	68.89	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.398		Crippen Method
mcvol	236.020	ml/mol	McGowan Method
pc	1726.03	kPa	Joback Method
rinpola	1936.00		NIST Webbook
rinpola	1936.00		NIST Webbook
tb	733.85	K	Joback Method
tc	935.72	K	Joback Method
tf	405.02	K	Joback Method
vc	0.887	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.37	J/molxK	733.85	Joback Method
cpg	722.50	J/molxK	767.50	Joback Method
cpg	739.47	J/molxK	801.14	Joback Method
cpg	755.29	J/molxK	834.79	Joback Method
cpg	769.98	J/molxK	868.43	Joback Method
cpg	783.56	J/molxK	902.08	Joback Method
cpg	796.05	J/molxK	935.72	Joback Method
dvisc	0.0017738	Paxs	405.02	Joback Method

dvisc	0.0008131	Paxs	459.82	Joback Method
dvisc	0.0004401	Paxs	514.63	Joback Method
dvisc	0.0002681	Paxs	569.43	Joback Method
dvisc	0.0001782	Paxs	624.24	Joback Method
dvisc	0.0001265	Paxs	679.05	Joback Method
dvisc	0.0000945	Paxs	733.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405240&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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