

Glutaric acid, di(1-phenylethyl) ester

Inchi: InChI=1S/C21H24O4/c1-16(18-10-5-3-6-11-18)24-20(22)14-9-15-21(23)25-17(2)19-12-7
InchiKey: BINGVWUXLVUIJH-UHFFFAOYSA-N
Formula: C21H24O4
SMILES: CC(OC(=O)CCCC(=O)OC(C)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 340.41

Physical Properties

Property code	Value	Unit	Source
gf	-121.96	kJ/mol	Joback Method
hf	-503.87	kJ/mol	Joback Method
hfus	36.76	kJ/mol	Joback Method
hvap	84.43	kJ/mol	Joback Method
log10ws	-5.46		Crippen Method
logp	4.765		Crippen Method
mcvol	274.110	ml/mol	McGowan Method
pc	1647.09	kPa	Joback Method
rinpol	2712.00		NIST Webbook
tb	884.94	K	Joback Method
tc	1111.88	K	Joback Method
tf	493.59	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	841.44	J/mol×K	884.94	Joback Method
cpg	901.46	J/mol×K	1074.05	Joback Method
cpg	892.01	J/mol×K	1036.23	Joback Method
cpg	881.33	J/mol×K	998.41	Joback Method
cpg	869.38	J/mol×K	960.59	Joback Method
cpg	856.10	J/mol×K	922.76	Joback Method
cpg	909.74	J/mol×K	1111.88	Joback Method
dvisc	0.0000402	Pa×s	884.94	Joback Method
dvisc	0.0000534	Pa×s	819.72	Joback Method

dvisc	0.0000746	Pa×s	754.49	Joback Method
dvisc	0.0001110	Pa×s	689.27	Joback Method
dvisc	0.0001794	Pa×s	624.04	Joback Method
dvisc	0.0003243	Pa×s	558.82	Joback Method
dvisc	0.0006858	Pa×s	493.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377518&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
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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