

Glutaric acid, di(2-phenoxyethyl) ester

Inchi: InChI=1S/C21H24O6/c22-20(26-16-14-24-18-8-3-1-4-9-18)12-7-13-21(23)27-17-15-25-1
InchiKey: BXYFAGKNDXOYLC-UHFFFAOYSA-N
Formula: C21H24O6
SMILES: O=C(CCCC(=O)OCCOc1ccccc1)OCCOc1ccccc1
Mol. weight [g/mol]: 372.41

Physical Properties

Property code	Value	Unit	Source
gf	-327.08	kJ/mol	Joback Method
hf	-757.75	kJ/mol	Joback Method
hfus	46.18	kJ/mol	Joback Method
hvap	90.02	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.401		Crippen Method
mvol	285.850	ml/mol	McGowan Method
pc	1582.23	kPa	Joback Method
rinpol	2949.00		NIST Webbook
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tb	930.66	K	Joback Method
tc	1152.50	K	Joback Method
tf	568.05	K	Joback Method
vc	1.079	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	894.98	J/molxK	930.66	Joback Method
cpg	907.76	J/molxK	967.63	Joback Method
cpg	919.05	J/molxK	1004.61	Joback Method
cpg	928.86	J/molxK	1041.58	Joback Method
cpg	937.21	J/molxK	1078.55	Joback Method
cpg	944.10	J/molxK	1115.53	Joback Method
cpg	949.56	J/molxK	1152.50	Joback Method
dvisc	0.0002630	Paxs	568.05	Joback Method

dvisc	0.0001495	Paxs	628.49	Joback Method
dvisc	0.0000939	Paxs	688.92	Joback Method
dvisc	0.0000635	Paxs	749.36	Joback Method
dvisc	0.0000456	Paxs	809.79	Joback Method
dvisc	0.0000342	Paxs	870.23	Joback Method
dvisc	0.0000267	Paxs	930.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376923&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

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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