

Glutaric acid, butyl 2,5-dimethylphenyl ester

Inchi: InChI=1S/C17H24O4/c1-4-5-11-20-16(18)7-6-8-17(19)21-15-12-13(2)9-10-14(15)3/h9-10
InchiKey: WAQHUAAMBVCCGZ-UHFFFAOYSA-N
Formula: C17H24O4
SMILES: CCCCOC(=O)CCCC(=O)Oc1cc(C)ccc1C
Mol. weight [g/mol]: 292.37

Physical Properties

Property code	Value	Unit	Source
gf	-282.43	kJ/mol	Joback Method
hf	-670.22	kJ/mol	Joback Method
hfus	38.62	kJ/mol	Joback Method
hvap	75.35	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	3.722		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1656.49	kPa	Joback Method
rinpol	2170.00		NIST Webbook
rinpol	2170.00		NIST Webbook
tb	777.58	K	Joback Method
tc	978.83	K	Joback Method
tf	477.13	K	Joback Method
vc	0.927	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	703.59	J/molxK	777.58	Joback Method
cpg	718.91	J/molxK	811.12	Joback Method
cpg	733.23	J/molxK	844.66	Joback Method
cpg	746.57	J/molxK	878.21	Joback Method
cpg	758.92	J/molxK	911.75	Joback Method
cpg	770.30	J/molxK	945.29	Joback Method
cpg	780.72	J/molxK	978.83	Joback Method
dvisc	0.0006671	Paxs	477.13	Joback Method

dvisc	0.0003993	Paxs	527.21	Joback Method
dvisc	0.0002612	Paxs	577.28	Joback Method
dvisc	0.0001829	Paxs	627.36	Joback Method
dvisc	0.0001350	Paxs	677.43	Joback Method
dvisc	0.0001039	Paxs	727.51	Joback Method
dvisc	0.0000827	Paxs	777.58	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358937&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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