

Succinic acid, dec-2-yl 4-chlorobenzyl ester

Inchi: InChI=1S/C21H31ClO4/c1-3-4-5-6-7-8-9-17(2)26-21(24)15-14-20(23)25-16-18-10-12-19
InchiKey: CKUKUWFNCQURLC-UHFFFAOYSA-N
Formula: C21H31ClO4
SMILES: CCCCCCCC(C)OC(=O)CCC(=O)OCc1ccc(Cl)cc1
Mol. weight [g/mol]: 382.92

Physical Properties

Property code	Value	Unit	Source
gf	-253.49	kJ/mol	Joback Method
hf	-762.33	kJ/mol	Joback Method
hfus	50.05	kJ/mol	Joback Method
hvap	87.59	kJ/mol	Joback Method
log10ws	-6.73		Crippen Method
logp	5.846		Crippen Method
mvol	310.110	ml/mol	McGowan Method
pc	1226.84	kPa	Joback Method
rinpol	2695.00		NIST Webbook
rinpol	2695.00		NIST Webbook
tb	901.11	K	Joback Method
tc	1109.38	K	Joback Method
tf	524.61	K	Joback Method
vc	1.194	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	964.82	J/molxK	901.11	Joback Method
cpg	1029.03	J/molxK	1074.67	Joback Method
cpg	1018.52	J/molxK	1039.96	Joback Method
cpg	1006.88	J/molxK	1005.25	Joback Method
cpg	994.07	J/molxK	970.53	Joback Method
cpg	980.06	J/molxK	935.82	Joback Method
cpg	1038.42	J/molxK	1109.38	Joback Method
dvisc	0.0000373	Paxs	901.11	Joback Method

dvisc	0.0000487	Paxs	838.36	Joback Method
dvisc	0.0000664	Paxs	775.61	Joback Method
dvisc	0.0000957	Paxs	712.86	Joback Method
dvisc	0.0001479	Paxs	650.11	Joback Method
dvisc	0.0002509	Paxs	587.36	Joback Method
dvisc	0.0004830	Paxs	524.61	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389680&Units=SI

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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