Glutaric acid, 2-acetyl-4-chlorophenyl butyl ester

Other names: Glutaric acid, 2-acetyl-4-chlorophenyl butyl ester
Inchi: InChI=1S/C16H19ClO5/c1-2-3-9-21-15(19)5-4-6-16(20)22-14-8-7-13(17)10-12(14)11-18/
InchiKey: NBAOXRVXXDQQFD-UHFFFAOYSA-N
Formula: C16H19ClO5
SMILES: CCCCOC(=O)CCCC(=O)Oc1ccc(Cl)cc1C=O
Mol. weight [g/mol]: 326.78

Physical Properties

Property code	Value	Unit	Source
hf	-877.40	kJ/mol	Cheméo Relay (1.0)
hfus	42.52	kJ/mol	Joback Method
hvap	93.34	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.20		Cheméo Relay (1.0)
logp	3.571		Crippen Method
mcvol	241.230	ml/mol	McGowan Method
rinpol	2441.00		NIST Webbook
tb	632.99	K	Cheméo Relay (1.0)
tc	857.69	K	Cheméo Relay (1.0)
tf	287.85	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	687.21	J/mol×K	840.79	Joback Method
cpg	745.05	J/mol×K	1050.94	Joback Method
cpg	737.85	J/mol×K	1015.92	Joback Method
cpg	729.69	J/mol×K	980.89	Joback Method
cpg	720.56	J/mol×K	945.87	Joback Method
cpg	710.44	J/mol×K	910.84	Joback Method
cpg	699.32	J/mol×K	875.82	Joback Method
dvisc	0.0001912	Pa×s	689.28	Joback Method
dvisc	0.0000908	Pa×s	840.79	Joback Method
dvisc	0.0001127	Pa×s	790.29	Joback Method
dvisc	0.0001442	Pa×s	739.79	Joback Method

dvisc	0.0006124	Pa×s	537.78	Joback Method
dvisc	0.0002650	Pa×s	638.78	Joback Method
dvisc	0.0003887	Pa×s	588.28	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U358933&Units=SI
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
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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point